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COM-75-11110

MASS SPECTRAL SEARCH SYSTEM

USER'S MANUAL

NATIONAL BUREAU OF STANDARDS

MAY 1974

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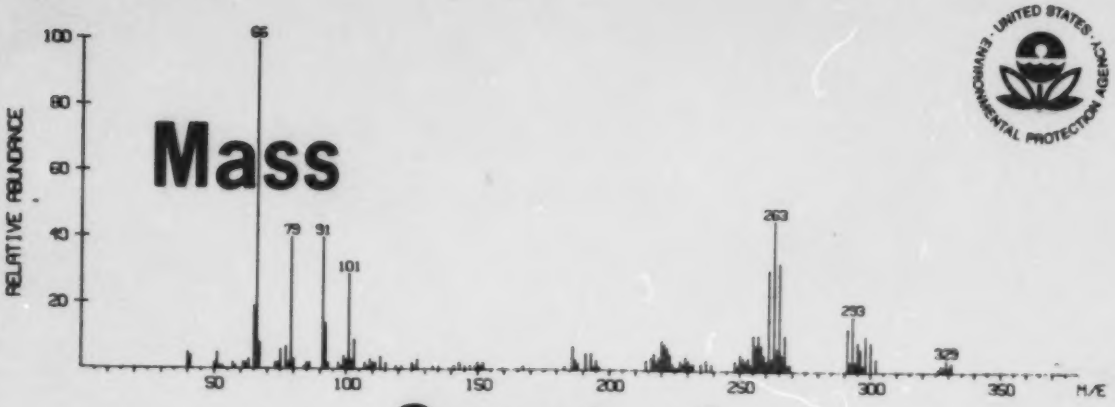
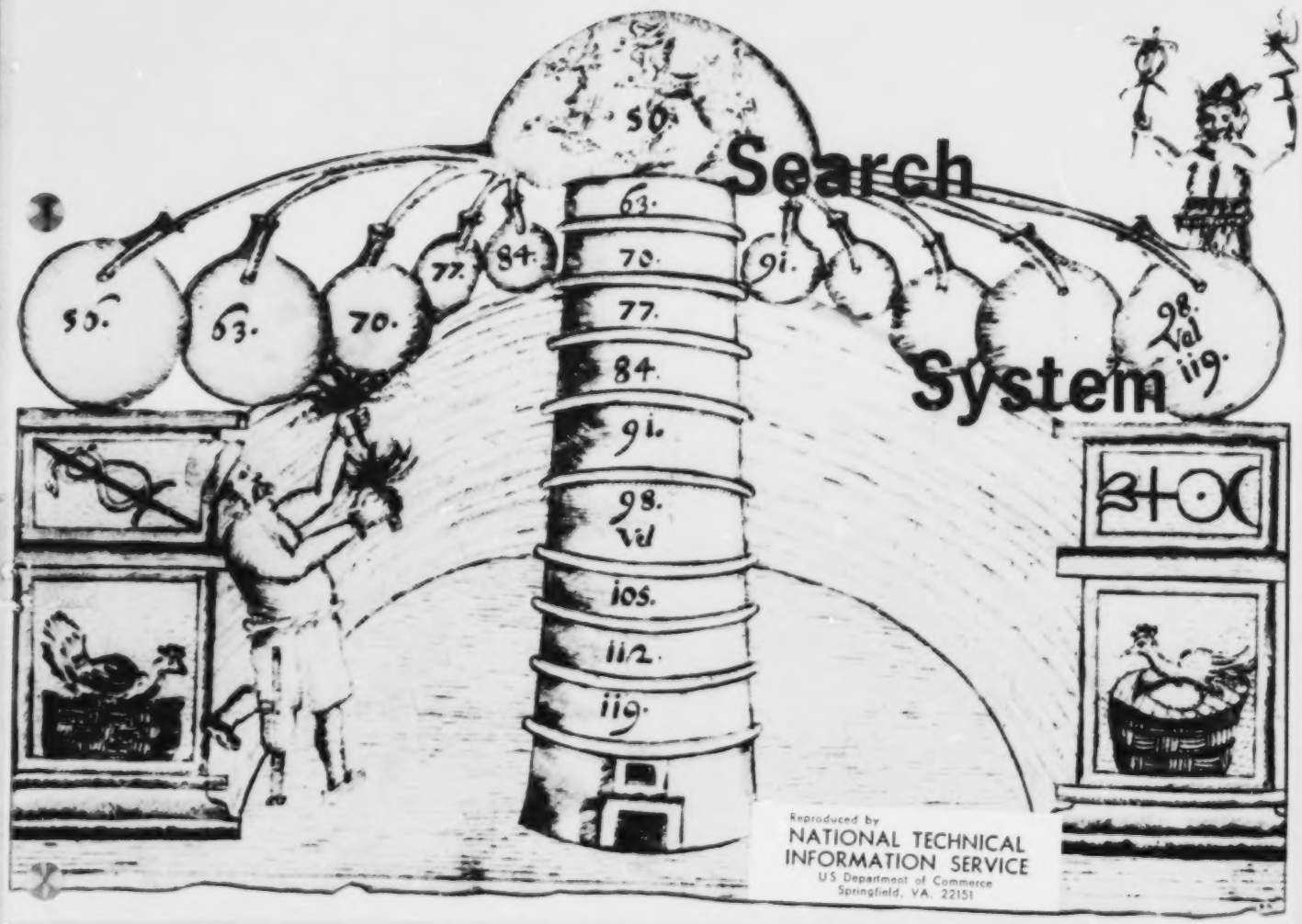
USERS MANUAL

MAY 1974



Mass Spectral Search System



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This manual explains all the various approaches to searches of the Mass Spectral Data base and gives examples to assist in understanding the options more clearly. The appraoches, such as using m/e values, losses from the molecular ion, MSDC codes, molecular formula (MF), and molecular weights (MW) result in the names of compounds in the file that meet the requested criteria.

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INTRODUCTION

The Mass Spectral Search System (hereafter referred to as MSSS) is a collection of programs to search rapidly and interactivly a large file of mass spectral data (currently 12,769 spectra) using a number of different approaches (see references 1-13 for details). The approaches, such as using m/e values, losses from the molecular ion, MSDC codes, molecular formula (MF), and molecular weights (MW) result in the names of compounds in the file that meet the requested criteria. The spectra themselves, may also be retrieved by using their ID#s, if desired.

The manual, now in its third edition, explains all the various approaches and options currently available and gives examples to assist in understanding the options more clearly. The first two editions were used in conjunction with an experimental MSSS on a PDP-10 computer in the Division of Computer Research and Technology (DCRT) at the National Institutes of Health (NIH), Bethesda, Maryland, USA. The project was sponsored by the National Heart and Lung Institute (NHLI) at NIH with the cooperation of the Mass Spectrometry Data Centre (MSDC), Aldermaston, Reading,

UK. The MSDC is an agency of the British government. The project was deemed successful, but since funding by NIH is limited to research activities, it was necessary to provide other means for the continuation of the MSSS. The MSDC contracted with General Electric (GE) to have the MSSS made available via the world wide GE Mark III Foreground System, available from local telephones currently on four continents. The United States government is assisting the British government in this non-profit, cost recovery venture by allowing the MSDC non-exclusive use of the software on the GE network. The MSSS is the responsibility of the MSDC and GE (in the US and Canada), Honeywell (in most of Western Europe and Australia), Dentsu (in Japan) and other authorized GE network distributors are acting only as marketing agents for the MSSS. The MSSS is still operational on the PDP-10 at NIH as well as the GE-635 on the GE network. The NIH system is available only to a limited number of scientists in the US federal government who have valid authorized accounts on the NIH computer. All other scientists use the GE MARK III Timesharing system. Details on obtaining accounts on both systems are given in Appendix A. Users of the GE MARK III Timesharing system currently pay a small initiation fee and modest yearly royalty fee for access to the system as well as the computer costs for each search. Note well, that the fees go to the MSDC, not to GE, nor NIH, nor the authors. The royalty fee is designed to minimize the deficit of the costs of the

system, which include, on-line disk storage of all data, software maintenance and additions, data base maintenance, corrections, additions, etc. The system has essentially a fixed overhead and thus the more users, the lower the royalty can be in the future.

This one manual is designed to be used on both operational systems. The only real differences between the them are the phone numbers and login procedures.

The system was designed for the user and the success that has been obtained is due mainly to feedback from the users. The current options and future options for searching as well as the size and quality of the data base are mainly dependent on the user. Only through their cooperation and assistance can the system fulfill the needs of the mass spectrometry community. Unless users send in new spectra, the file cannot grow! Information regarding who to contact about specific information is given in Appendix B.

The system has been supported and assisted by many groups and individuals. Of particular note are the following:

Mass Spectrometry Data Centre (MSDC)
National Institutes of Health (NIH)
Environmental Protection Agency (EPA)
General Electric Co. (GE)
North Atlantic Treaty Organization (NATO)
Department of Trade and Industry (DTI)

Dr. K. Biemann (MIT)
Ms. A. Bridy (NIH)
Mr. T. Choate (GE)
Dr. N. Daly (MSDC)
Dr. H. Fales (NIH)
Mr. R. Feldmann (NIH)
Ms. R. Heller (University of Maryland)
Dr. S. Heller (EPA)
Ms. C. Kenney (NIH)
Ms. D. Koniver (NIH)
Mr. D. Maxwell (MSDC)
Dr. A. McCormick (MSDC)
Dr. J. McGuire (EPA)
Mr. L. McNeil (GE)
Dr. G. W. A. Milne (NIH)

A MSSS advisory committee has been established to overlook and coordinate efforts. The current committee members are from the staffs of MSDC, EPA, NIH, University of Maryland and GE.

PDP-10 LOGIN

At present the DCRT/CCB PDP-10 has a number of methods by which one can access the machine. The simplest are the teletypes or Datapoints (Cathode Ray Tube "teletypes") which are located at the PDP-10 in the basement of Building 12A and in other areas in Building 12A. Next there are a number of telephone lines which can be dialed up from terminals from any laboratory at NIH, any laboratory in the Washington D.C. area, or in fact, from any where in the world (assuming you have the correct telephone attachment or "modem" on your terminal).

The PDP-10 is a 36-bit word, ASCII machine. The telecommunications lines at the computer use the standard Bell System 103A modems. Terminals using modems or acoustic couplers should transmit or send at a mark frequency of 1270 Hz. and a space frequency of 1070 Hz. and should receive at a mark frequency of 2225 Hz. and a space frequency of 2025 Hz. N.B.: These are Ma Bell (AT&T) frequencies found almost exclusively in the USA. In Europe and elsewhere, contact your local GPO or PTT for further technical information and regulations regarding acoustic couplers and CCITT modems.

The most common terminal is the standard teletype, known as the Model-33 teletype. The PDP-10 can be reached from this terminal by dialing: 301-654-6883 (This is not an FTS phone number and there are no 10 cps FTS phone lines to the PDP-10.) This line is a rotor which links (at present) to ten other lines. The teletype should be set at "full-duplex". If there is no switch or provision for this (which is indicated by the terminal producing double sets of letters, e.g., LLOOGG), then as soon as you have contacted the PDP-10 computer, you should type "TTY NO ECHO", which appears as "TTTTYY NNOO EECCHHOO" when you type it. Sometimes this must be repeated several times before it works. In case there is no response when you type "LOG", type "TTY ECHO" and things should be fine.

If you have a terminal which has variable speed lines, you may want to use a telephone line that will transmit at 30 characters/second vs. the 10 characters/second for the standard teletype. These are such terminals as the Texas Instruments models 725 and 733, the Computer Devices model 1030 and the Execuport models 300 and 310. The number for the high speed line is 301-656-4261. (This is not an FTS phone number and there are no 30 cps FTS phone lines to the PDP-10.) The line is also an eight line rotor.

One step up from the 30 cps line is the 120 cps line, for such terminals as the Tektronix 4000 series. The single 1200 baud phone line for the PDP-10 requires a Vadic modem to work properly. The telephone number for the 1200 baud (120 cps) line is 301-657-3080. It is not an FTS phone number and there are no 120 cps phone lines to the PDP-10 that use just one phone line.

Lastly, the PDP-10 can be dialed up from the IBM Selectric terminals, the IBM 2741 and Datel 707. There is currently only one telephone line for this type of terminal, whose number is 301-496-6169. There will be more lines added in the near future. Internally at NIH one can get to the PDP-10 by dialing 3 if you have a selectric 2741 terminal attached to a dataphone. The 2741 was NOT designed to operate with the PDP-10. However, the PDP-10 system's team has "patched" around many of the 2741's inadequacies for use on the PDP-10 and it can be used for the mass spectral search system. However, it has been found that the 2741 terminal gets hung, drops transmission characters, etc. -- so beware!!!

Please note that the telephone numbers may change as the system is modified, so that if you have any problems with contacting the computer, or you want to check and see

if the computer is "up" or "down", please call 301-496-6755. However, if you have any difficulties with the search system, please see Appendix B or use the CRAB program.

After the terminal is properly hooked up to the computer, hit the carriage return (CR) once or twice and then after getting a response of ".", type "LOG" followed by a carriage return (CR). Sometimes you will first get "? LOGIN PLEASE" typed back to you before you get the ".". The computer will respond with a request for your number, which is 1543,7643 in the example below. Then the computer will request your password, which is to be given followed by a carriage return. (The computer does not print the password even tho you are typing it). The reason for this is that the signal you are "typing" really goes first to the computer, where it is interpreted and then echoed back to you by the key striking the paper. You may think you are actually typing the letters as you strike the key, but you aren't!! This should explain the TTY NO ECHO and TTY ECHO statements above. The computer will then respond with a period, indicating the monitor is "listening" to you. You then type CHEM followed by a carriage return again to call up the DCRT/CIS (Chemical Information System) Administration Program. This program directs you to use any of the programs under development in the system and will vary from time to time as the CIS develops and evolves. (Sometimes you may find the login routine a little different, for

example the CHEM Administration Program may be started up automatically). The following example is a teletype style login.

This new manual also includes the changes in the dialog from the previous version. The shortening of the dialog is in response to many users with 10 cps (110 baud) teletype type terminals which seem to take forever to type out. Hopefully, there remains enough dialog so that the system is still easy to use.

The part of the dialog that you type or insert is underlined in this text and is usually preceded by a ":" or ".". Every response must be followed by a carriage return, abbreviated as "CR".

```
.LOG
JOB 14 DCRT/CCB 507 DUAL PROCESSOR TTY2
#1543,7643
PASSWORD:
0921 05-JAN-74  SAT
OTHER JOBS SAME PPN
NO MAIL
.
```

```
.R CHEM

CHEM
DCRT/CIS CHEMICAL INFORMATION SYSTEM

TO RUN A PROGRAM IN THE CIS, TYPE THE NUMBER NEXT TO THE NAME
OF THE PROGRAM

LITERATURE:

CBAC - 1

STRUCTURE:

SUBSTRUCTURE SEARCH - 2      WLN GENERATION - 3
WLN TO STRUCTURE - 4     WLN GENERATION USING THE TABLET - 17

DATA:

MASS SPEC - 5     NMR - 6

ANALYSIS:

XYZ COORDINATE GENERATOR - 7     XRAY COORDINATE REFORMAT - 8
XRAY MODELING SYSTEM - 9    XRAY CRYSTAL BIBLIO SYSTEM - 10
CNDO/INDO - 11    MINDO - 12    ORTEP -13
GINA NMR ANALYSIS - 14    ESR SPECTRUM SIMULATION - 15
MLAB CURVE FITTING/MODELING - 16

USER CHOICE: 5
DOING THE OVERLAY
```

After typing 5 (CR) for requesting the mass spec search system program to be fetched and run, the program will first request your name and address and then request a set of initials, and you respond with three (3) initials. The program responds and asks if you want the choices available typed out. The need for the initials is to keep each user of the system from disturbing any other user. The choices are printed only once if you want as you enter the search system. After the first time the system responds just with the request: "USER RESPONSE:". For example:

```
DCRT/CIS - NHLI MASS SPECTRAL SEARCH SYSTEM

READ THE NEWS OF 3/1/74

YOUR NAME AND COMPANY PLEASE

USER: STEPHEN R. HELLER, EPA, WASHINGTON, D.C. 20460

YOUR 3 INITIALS PLEASE

USER:SRH

TO LIST SEARCH OPTIONS, TYPE OPT, CR TO CONTINUE

USER: OPT

TO SEARCH FOR PEAKS, TYPE PEAK
TO SEARCH FOR LOSSES, TYPE LOSS
TO SEARCH FOR MSDC CODES, TYPE CODE
TO SEARCH FOR MOLECULAR FORMULA, TYPE MF
TO SEARCH FOR MOLECULAR WEIGHT, TYPE MW
TO SEARCH FOR PEAKS AND LOSSES, TYPE PL
TO SEARCH FOR PEAKS WITH MF, TYPE PMF
TO SEARCH FOR PEAKS WITH MW, TYPE PMW
TO SEARCH FOR PEAKS WITH MSDC CODES, TYPE PC
TO SEARCH FOR LOSSES WITH MSDC CODES, TYPE LC
TO SEARCH FOR LOSSES WITH MF, TYPE LMF
TO SEARCH FOR LOSSES WITH MW, TYPE LMW
TO SEARCH FOR MSDC CODES WITH MW, TYPE CMW
TO SEARCH FOR MSDC CODES WITH MF, TYPE CMF
TO SEARCH FOR MW WITH MF, TYPE MWMF
TO PERFORM A SIMILARITY COMPARISON, TYPE SIM
TO PRINT OUT PEAKS/INTENSITIES AND SOURCE, TYPE SPEC
TO PLOT SPECTRA ON DISPLAY TERMINAL, TYPE PLOT
TO VIEW MICROFICHE, TYPE FICHE
TO COMMENT/COMPLAIN, TYPE CRAB
TO READ THE NEWS OF THE SYSTEM, TYPE NEWS
TO LIST THE MSDC CODES, TYPE LIST
TO ENTER NEW SPECTRA, TYPE DATA
TO EXIT FROM THE PROGRAM, TYPE OUT

USER:
```

If you type OUT, that will exit you from the program, but not from the computer.

```
USER RESPONSE:OUT

CPU TIME: 11.50 ELAPSED TIME: 13.11.40
NO EXECUTION ERRORS DETECTED

EXIT
```

To terminate the job in the computer, type "LOGOUT" or "K/P". The computer will respond as shown below.

```
.LOGOUT
JOB 14, USER (1543,7643) LOGGED OFF TTY2 1030 05-JAN-74
SAVED ALL FILES (70 BLOCKS)
RUNTIME 0 MIN, 13.12 SEC

OR


.K/P

OTHER JOBS SAME PPN
 JOB 14, USER (1543,7643) LOGGED OFF TTY2 1005 05-JAN-74
ANOTHER JOB STILL LOGGED IN UNDER [1543,7643]
RUNTIME 0 MIN,  24.45 SEC
```

Occassionally there may be an error or problem in running the program, due to some temporary software or hardware failure (often found when you are doing an MF search). If you get an error such as:

?ERROR IN JOB 14 ?ILLEGAL UUO AT USER 020232

Just start up the program again by typing: "R CHEM".

To supress printout from the PDP-10, you can type control O (↑O) which is done by holding down the control key on the terminal and hitting the O key. The results looks like this: "↑O". To return to the monitor (i.e. a quick and dirty way to exit from the program), type control C (↑C).

GE INTERNATIONAL NETWORK LOGIN

THE MARK III FOREGROUND COMPUTER SERVICE

MSSS resides on a modern, large-scale computer. NONE of the other CIS programs (Xray, SSS, NMR, etc.) listed in the PDP-10 login in the previous section are now available in the GE MARK III Foreground system. This system, known as MARK III Foreground, is totally dedicated to the interactive, time-sharing user. MARK III is compatible with almost any terminal using ASCII or EDCDIC code sets at rates of 10, 13.5, 15, and 30 characters per second. Connecting the MSSS user with the MARK III service is a world-wide communications network, which permits MARK III access via a local telephone call from over 350 cities in the USA, Canada, Japan, Western Europe, and Australia.

Supporting this MARK III network is a sales and support organization of over 50 General Electric Information Services offices throughout the United States. Each office is staffed with people who will help the user with systems or programming problems.

An International Access Directory lists all United States computer access numbers, plus the nearest General Electric Customer Service Desk. These Directories are available from your General Electric Information Services office at no charge (see Appendix A). The telephone numbers (as of January 1974) from this directory are given in Appendix C.

ACCESSING MSSS ON MARK III

Let's assume that you have the common Teletype Model 33 terminal (ASR 33), and that it can be connected to a telephone line via an acoustic coupler (a small, box-like receptacle which has recesses for the telephone's handset). The proper acoustic coupler (if legal to use in your country) or modem can be obtained from various commercial sources or your local PTT government telephone system.

NOTE: Except for the first entry, the H (which tells the computer what type of terminal you are using), follow each typed entry with a carriage return (CR).

The access procedure is as follows:

1. Make sure that the acoustic coupler is set for half duplex (not full duplex, which is used on the PDP-10).

2. Dial the local General Electric computer access number (See Appendix C), and wait for the high-pitched tone, which indicates contact with the network has been established.

3. Place the telephone handset firmly in the coupler, and type an H.

4. The terminal will print out:

   U#=

   in response to which you type your user number, (The catalog in which the MSSS resides originally was GAQ48, later changed to KAQ48 and is currently (March 1974) LAQ48. Thus the login example will be of a general nature.) For example:

   ABC99001, (CR)

   The terminal will now print:

   PASSWORD

   MMMMMMMM You type your password in this masked area and CR. If you have accidently mistyped your user number and password, the terminal will type:

   INCORRECT FORMAT, RETYPE IT-- Retype your user number here. The computer then asks for your ID, and you give your ID, followed by a CR.

   ID:

5. Upon successful completion of this access sequence (or "logon", as this procedure is often called), there will be a slight pause, and then the terminal will print:

```
ALDERMASTON/NIH   MASS SPECTRAL SEARCH SYSTEM
READ THE MARCH NEWS
TO LIST SEARCH OPTIONS, TYPE OPT, CR TO CONTINUE
USER:  (CR)
PUBLIC (PUB) OR PRIVATE (PRI) FILE  ??
USER:PUB
```

Any other special messages concerning the system's operation will be printed automatically.

6. Having printed the title banner and any news of interest to the MSSS user, the MARK III system will then commence the execution of the MSSS computer program. Those users who logged on to use other features of the MARK III system, such as its extensive applications library or user written programs, may exit from the MSSS program by typing OUT after the options are listed.

5. When you are finished with your searching, you exit from the program by typing "OUT", and then to logout, type "BYE". For example:

```
USER RESPONSE:OUT

PROGRAM STOP AT 0

USED     16.21  UNITS

BYE

0016.21 CRU    000.47 TCH    0000.89 KC

OFF AT 20:38EDT  01/05/74
```

Occasionally there are systems problems on GE (usually at the beginning of the month or after a weekend reloading of the system) and you may get the following message printed out:

```
      ERROR IN LINE CALLING ROUTINE
```

or

```
LOAD ABORT .OPENFILE      TWELVE
LINE CALLING ROUTINE
0    CHEM$$
```

```
PROGRAM STOP AT 1120
```

If this occurs, type "RUN CRAB$$" or call your local GE MARK III Timesharing System office. Once the program is reloaded, the MSSS will be available again.

SOME MARK III SYSTEM COMMANDS OF INTEREST TO THE MSSS USER

While not an exhaustive list of the commands available to the MSSS user, the following list of system commands should assist those who plan to use the MARK III Service for other purposes, such as using the MARK III applications program library, containing over 500 programs, or writing and executing their own programs. For a complete description of all system commands, refer to the Command System manual, GE publication number 3501.01. This manual is available through your local GE MARK III Timesharing System office.

NOTE: Any of the following commands may be typed in whenever MARK III has just terminated a program's execution, or when it has just typed a READY on the previous line. All system commands may be abbreviated to the first three letters for each entry.

ACTIVITY Causes MARK III to print out the number of computer resource units used during the current session since logon.

BYE — Causes the end of the MARK III session and a disconnect.

CATALOG — Lists the names and dates last accessed of all files stored within stored within the user's private library (such as his proprietary mass spec files).

LIST — Causes MARK III to print out the contents of the current data file or program. LIST--130 causes the printing to start with line 130.

NEW — Tells MARK III that a new file is about to be entered. You must use the REPLACE or SAVE command to have MARK III retain the file after log-off.

OLD — Tells MARK III that the filename following the OLD command has been previously SAVED (or REPLACED) in the computer, and moves it into current working storage

PROJECT — Causes MARK III to associate all further use during the current session with a new Project Identification. This command is only for users validated for Project ID feature.

RUN — Causes the execution of a program. If entered after a program execution has commenced, but while the terminal is not printing, MARK III will print out the computer resource unit expended thus far in the execution.

STATUS — Causes MARK III to inform you of the last command it received (but which has not been completed).

TTY — Causes MARK III to inform you of access port number, user number, name of file in current storage, compiler in use, and execution status.

UNSAVE — Causes MARK III to erase the permanent copy of the file in current storage. (PURGE may also be used for the same purpose).

OBTAINING USAGE INFORMATION FROM MARK III (for USA customers only)

The MSSS user is offered the capability of determining costs accrued on a previous-month basis, or a month-to-date basis. This capability is available through the execution of a permanent program named COSTS$.

To executive COSTS$, merely type RUN COSTS$ (followed by a carriage return). The only other interaction required with the computer is to respond to the question asking whether you want last month's data or the current month's. COSTS$ does the rest, determining and displaying usage information and related dollar values for all interactive MARK III usage for the period requested. There is no charge for the provision of this capability, other than the computer execution time required to execute the COSTS$ program.

PEAK AND INTENSITY SEARCH

The peak and intensity search option module, normally referred to as the peak search is the most commonly used option in the system. The peak search does NOT search the file of complete spectra, but rather a file of abbreviated spectra. The original abbreviation was to select the two most intense peaks in every 14 amu interval, starting at an m/e of 6. The file now being searched contains the THREE (3) most intense peaks in every 14 amu interval, starting at an m/e of 6. The change from 2 out of 14 to 3 out of 14 was to reduce cases of non hits from searching and is based on previous experience with the system. The intervals used are:

6-19,20-33,34-47,48-61,62-75,76-89,90-103,104-117,
118-131,132-145,146-159,160-173,174-187,188-203, etc.

Please note these intervals carefully when you choose your peaks; it is pointless to choose more than three from any of the above 14 AMU intervals! If you must choose 3 in a 14 amu interval because of paucity of data, etc., make sure that they are divided by one of the above intervals, i.e. 145,146,147 would be allright.

The program further reduces the number of possibilities by using the intensity of the peak to reject peaks that are too big or too small. Because of instrumental variations an intensity range factor has been built into the program. The range is variable and is determined every time you use the program. A good starting range factor is 3 or 4. Remember to check that the peak you are entering is one of the three largest from that 14 m/e mass interval. Please note that there are NO metastable peaks in the file. Doubly-charged ions are also not included unless they have an integral mass and happen to be
unusually intense.

The peaks in the abbreviated search file range from m/e of 8 to m/e of 1330. The ten most common peaks in this abbreviated file are:

m/e	# Refs	m/e	# Refs
41	7177	29	5878
27	6755	55	5576
39	6263	77	4707
43	5997	69	4670
28	5879	57	4342

The abbreviated file contains 358,194 peaks out of the 1,019,369 peaks in the complete file (i.e., 35.14 %).

The intensities of the peaks in the computer file range from 0 to 100, i.e 0.0 to 100.0 %. The 0 -100 range was obtained from 0-9999 (see format in Appendix E) by adding 50 and dividing by 100. The intensity range factor is used to multiply and divide the intensity value you give to determine the range or window size to be used. For example, an intensity factor value of 4 and an intensity of 40% will result in all peaks with intensities >10% and <100%(really 160%, but 100% is the maximum value) being selected. If the value was 2 and the intensity 40, then all peaks with intensities >20% and <80% will be selected. The intensity range factor can be used in a number of ways. If the range factor is 100 or greater, then there will be no intensity filtering, since 100 times any intensity and any intensity divided by 100 will include the range of 0 to 100. To look at the high intensity peaks, a range factor of 2 and an intensity of 150 (150.0 %) will allow only peaks with an intensity greater than 75% to be passed out as a possible answer. It is important to note that the range factor must be an integer, thus 1.5 is a no-no. If you don't put in an intensity range factor, but rather just hit the carriage return (CR), the program will automatically set the factor

at 4. Note that the range factor allows for a rather wide variation on large peaks, but small ones are much more restricted. Thus a compound in the file having a small molecular ion of say 2%, while it might well be the largest ion in its 14 AMU group, would be missed by using a range factor of 2 if it happened to be as high as 5% as run on your spectrometer. One way around this specific problem would be to enter the molecular ion as the molecular weight (MW) in the combination search option, peak and molecular weight (PMW). See page 44 for details of this option.

One possible solution to this is to change the procedure for entering the range from a factor (as it is now) to an actual range. For example, 100,1,7 would be interpreted by the program as a peak at mass 100, with an allowable intensity of 1% to 7% and 134,40,100 would mean a peak at mass 134 with an allowable intensity between 40% and 100%. This method may be implemented in the future if users feel it would be a better way to search for peaks. Speak up if you want to be heard!

After giving the program the intensity range factor, you will be asked for peaks and intensities, one mass and intensity at a time. The computer then responds with the number of spectra out of the entire file of 12,769 spectra that meet the requirements specified for the mass and intensity range. If you care, you can have the answers

typed out. Most of the time you will need to enter a few (2-4) peaks before the search procedure narrows down the number of spectra meeting your requirements to a reasonable number (5-10) spectra out of the 12,769 spectra. After entering the second mass and intensity, and for all peaks and intensities thereafter, the program automatically finds all those spectra that contain that combination of peaks and intensities. If no spectra are found to contain the combination of peaks and intensities, then the prograr tells you this and allows you to go back one step and list the references from that step, or to continue on from that previous point. Again, at any point along the way you have the option to print the ID number and name of those compounds meeting your criteria of peaks and intensities. To increase the efficiency of the search, it is generally best to enter the highest masses first, provided they have reasonable intensity since the number of peaks at high masses tend to be smaller. This is satisfactory provided that the exact compound is in the file, but if if is not, this method may fail to locate an interesting lover homolog or related compound with a similar fragmentation pattern. If you type an incorrect peak or intensity value, restart the peak search program. The following pages are some examples of the peak and intensity search program.

PEAK AND INTENSITY SEARCH

USER: INTENSITY RANGE FACTOR IS: 2

TYPE PEAK,INT
CR TO EXIT, 1 FOR ID,MW,MF AND NAME

USER:85,100

# REFS	M/E PEAKS
214	85

NEXT REQUEST: 128,20

# REFS	M/E PEAKS
11	85 128

NEXT REQUEST: 29,30

# REFS	M/E PEAKS
8	85 128 29

NEXT REQUEST: 1

ID#	MW	MF	NAME
1671	170	C10.H18.O2	GAMMA–DECALACTONE
1688	254	C16.H30.O2	GAMMA–PALMITOLACTONE
1689	282	C18.H34.O2	GAMMA–STEAROLACTONE
6731	128	C8.H16.O	4–OCTANONE
6736	128	C8.H16.O	2–METHYL–3–HEPTANONE
6740	128	C8.H16.O	2–METHYL–4–HEPTANONE
6747	128	C8.H16.O	2,5–DIMETHYL–3–HEXANONE
8699	314	C19.H38.O3	METHYL 4–HYDROXYOCTADECANOATE

PEAK AND INTENSITY SEARCH

USER: INTENSITY RANGE FACTOR IS: 2

TYPE PEAK,INT
CR TO EXIT, 1 FOR ID,MW,MF AND NAME

USER:135,80

# REFS	M/E PEAKS
171	135

NEXT REQUEST: 150,40

# REFS	M/E PEAKS
28	135 150

NEXT REQUEST: 91,20

# REFS	M/E PEAKS
16	135 150 91

NEXT REQUEST: 57,20

# REFS	M/E PEAKS
2	135 150 91 57

NEXT REQUEST: 1

ID#	MW	MF	NAME
625	150	C10.H14.O	THYMOL
3446	204	C14.H20.O	P-TERT-BUTYLPHENYL METHALLYL ETHER

LOSS AND INTENSITY SEARCH

The loss and intensity search, commonly called the loss search, is simply a search for loss of some fragment (it might be a molecule,radical or ion) from the molecular ion. The file consists of losses from 0 (i.e. molecular ion) to -150 (i.e., M-150) whose intensities are 1% or greater. There is NO abbreviated file in this option. The only cutoff is 1% for intensity; one may not search for losses of fragments of mass 151 or greater no matter what these intensities are. There are 607,503 peaks in the loss file, which amounts to 59.60 % of the entire file.

In the search for losses, the input losses are preceded by a - sign and are negative numbers, with intensities, e.g. -15,30. This means a loss of 15 with an intensity of 30 of the resulting ion (not the molecular ion) multiplied and divided by whatever the intensity range factor you specify. The following example should explain the option clearly. For determining M in the case of isotopes (e.g. Br,Cl, etc.) use the lower mass isotope in calculating M. Thus the MW of HBr is 80.

Statistics of losses with more than 6500 occurrences in the file of 12,769 spectra

LOSS	# REFS
0	10822
43	7776
29	7581
57	7424
15	7398
71	7072
45	6686
28	6621
1	6595
44	6545
56	6508

As can be readily seen, the ion series 29,43,57,71 is extremely common and should be used only after a more interesting and useful loss is investigated.

LOSS AND INTENSITY SEARCH

USER: INTENSITY RANGE FACTOR IS: 4

TYPE LOSS,INT
1 TO EXIT, 2 FOR ID,MW,MF AND NAME

USER:-47,40

# REFS	LOSSES
904	-47

NEXT REQUEST: -65,30

# REFS	LOSSES
50	-47 -65

NEXT REQUEST: -31,40

# REFS	LOSSES
8	-47 -65 -31

NEXT REQUEST: 2

ID#	MW	MF	NAME
159	92	C3.H8.O3	GLYCEROL
498	110	C7.H10.O	3-METHOXY-1,3,4-HEXATRIENE
1491	106	C4.H10.O.S	(2-HYDROXYETHYL) ETHYL SULPHIDE
2190	106	C4.H10.O3	1,2,4-BUTANETRIOL
7523	104	C5.H12.O2	NEOPENTYLGLYCOL
8717	328	C20.H40.O3	METHYL 18-METHOXYOCTADECANOATE
9762	104	C5.H12.O2	NEOPENTYL GLYCOL
10747	326	C20.H26.N2.O2	VINCAMINOL

PEAK/LOSS AND INTENSITY SEARCH

This option is simply a combination of the peak search and the loss search modules. The rules for both hold for the combination. The peaks are the most intense 3/14 and the losses are >1% and go from M to M-150. In the following example two peaks and one loss were entered to to obtain the 5 references found.

PEAK AND LOSS SEARCH

USER: INTENSITY RANGE FACTOR IS: 2

TYPE PEAK OR LOSS, INT
2 TO EXIT, 1 FOR ID,MW,MF AND NAME

USER: 142, 190

# REFS	PEAKS/LOSSES
31	142

NEXT REQUEST: 0,190

# REFS	PEAKS/LOSSES	
23	142	0

NEXT REQUEST: -15,20

# REFS	PEAKS/LOSSES		
5	142	0	-15

NEXT REQUEST: 1

ID#	MW	MF	NAME
76	142	H8.BR.B5	BROMOPENTABORANE
2615	142	C.H3.I	IODOMETHANE
4539	142	C.H3.I	IODOMETHANE
5756	142	C8.H14.S	CIS-3-THIABICYCLO(4.3.0)NONANE
(CIS-5-THIAHEXAHYDROINDAN			
6456	142	H8.BR.B5	BROMOPENTABORANE

MOLECULAR WEIGHT SEARCH

The molecular weight search program searches for a given molecular weight in the file and responds either with the number of spectra with that molecular weight, or tells you that that particular molecular weight is not in the file. In the file of 12,769 spectra there are over 600 different molecular weights. These molecular weights range from 2 to 1520. If the program does find some compounds with a given molecular weight , you have the option of typing out the ID and names of those compounds. Sometimes it is useful to try a molecular weight of 14, 16, 28, 42, etc. mass units more or less, in the hope of identifying a homolog or metabolite, etc. A carriage return exits you from the molecular weight search and returns you to the main program for your next choice. For example:

MOLECULAR WEIGHT SEARCH

TYPE MW, CR TO EXIT

USER:113

FOUND 17 SPECTRA WITH MW: 113

LIST REFERENCES, YES OR NO?

USER:YES

ID#	MW	MF	NAME
181	113	C5.H4.N.CL	2–CHLOROPYRIDINE
182	113	C7.H15.N	2,3–DIMETHYLPIPERIDINE
313	113	C5.H7.N.S	3–BUTENYL ISOTHIOCYANATE
1001	113	C7.H15.N	2–ETHYLPIPERIDINE
1002	113	C5.H7.N.O2	ETHYL CYANOACETATE
2242	113	C5.H4.N.CL	3–CHLOROPYRIDINE
2243	113	C7.H15.N	CYCLOHEXYLMETHYLAMINE
5191	113	C7.H15.N	2,6–DIMETHYLPIPERIDINE
7063	113	C6.H11.N.O	CAPROLACTAM
7064	113	C6.H11.N.O	CYCLOHEXANONE OXIME
7065	113	C7.H15.N	N–ETHYLPIPERIDINE
7066	113	C6.H11.N.O	6–METHYL–2–PIPERIDONE
7355	113	C6.H11.N.O	2–METHYLAMINO–2–PENTEN–4–ONE
7526	113	C7.H15.N	N–METHYL CYCLOHEXYLAMINE
7761	113	C5.H7.N.O2	N–METHYLSUCCINIMIDE
9760	113	C7.H15.N	N–METHYLCYCLOHEXYLAMINE
12244	113	C2.H6.N.F2.P	DIMETHYLAMINODIFLUOROPHOSPHINE

MOLECULAR FORMULA SEARCH

The molecular formula search is really two separate search modules. The first is the usual search for a complete molecular formula, such as "C6.H6.O2" (periods are added to separate the atom types). In the file of 12,769 spectra there are over 4400 different molecular formula. The second is an imbedment molecular formula, which contains two types of atom groups. The first is the exact atom type and the second the stripped atom type. (These designations and this search option have nothing to do with mass spectra per se. They are useful only to find what spectra in the file contain a particular element or atom type.) The exact atom type is that quantitative part of a complete molecular formula (see example below). The stripped formula is the qualitative part of a complete molecular formula. For example, "C6.H6.O" is a complete, every day, run of the mill, molecular formula. "C6" is an imbedded molecular formula and one of three imbedded in "C6.H6.O" That is, the "C6" group is part of the complete molecular formula of the molecular (parent) ion.

To summarize the 3 MF searches we have:

1. All or complete
2. Qualitative: C,H,N,O, etc.
3. Quantitative: C_n,H_m,N_o,O_p, etc.

For an example of a search that shows the difference between the qualitative and quantitative searches, see pages 47-48 in the peak and partial formula search option.

The molecular formula information stashed away in the computer looks this way:

For the molecule "C6.H6.O" we have:

1.	Complete Formula:	C6.H6.O
2.	Partial Formula:	C6
		H6
		O1
3.	Stripped Formula:	C
		H
		O

For the molecule "C.H3.F3.SI" we have:

1.	Complete Formula	C.H3.F3.SI
2.	Partial Formula:	C1
		H3
		F3
		SI1
3.	Stripped Formula:	C
		H
		F
		SI

As you can see from these examples all carbon compounds have the same stripped formula "C", but their imbedded carbon formula can be, and usually are, different.

Statistics on the stripped partial formula
from the file of 12,769 mass spectra

C	12,651	F	572
H	12,424	Br	376
O	7329	Si	222
N	2743	B	189
Cl	1248	P	137
S	1138	I	100

Because most computer terminals are UPPER CASE only, the molecular formula file has a particular format that must be followed to find a compound. The ordinary scheme is: C, H, N, O, S, halogens (F,CL,BR,I) and then alphabetical. All complete molecular formula have a "." (period) between atom groups, except at the end of the formula. If you are looking for a formula C6.H6.O in the complete MF search, type "C6.H6.O" (and not "C6.H6.O1"). If you are looking for this molecule in the imbedded search, you type these groups: "C6", "H6" and "O1". (Note there are no "." in this search.) The "O1" as opposed to just "O" is to distinguish it from the stripped formula "O". Typing just "O" will not ruin the search, you will just get more answers than with an "O1" search. Both the searches for the imbedded and stripped MF are in the imbed search part of the MF option. The following examples should clarify the search procedure. Note that 0 (zero) and O (the letter "O") are different, so please check which key you are hitting!

MOLECULAR FORMULA SEARCH

TO SEARCH FOR A COMPLETE MF, TYPE ALL
TO SEARCH FOR A PARTIAL MF, TYPE IMBED
CR TO EXIT

USER:IMBED

USER: THE NUMBER OF ATOM TYPES IS: 3

USER: TYPE 1 IS:C6

USER: TYPE 2 IS:H6

USER: TYPE 3 IS:O2

FOUND 15 REFERENCES TO THAT COMBINATION

LIST REFERENCES, YES OR NO?

USER:YES

ID#	MW	MF	NAME
179	110	C5.H6.O2	5–METHYL–2–FURALDEHYDE
297	138	C6.H6.N2.O2	DI (ACETYL CYANIDE)
452	110	C6.H6.O2	CATECHOL
453	110	C6.H6.O2	RESORCINOL
454	110	C6.H6.O2	HYDROQUINONE
2212	110	C6.H6.O2	HYDROQUINONE
2214	110	C6.H6.O2	PYROCATECHOL
2216	110	C6.H6.O2	RESORCINOL
2217	110	C6.H6.O2	FURYL METHYL KETONE
2221	110	C6.H6.O2	2–FURYL METHYL KETONE
3170	180	C6.H6.O2.CL2	X–METHYL–X,X–DICHLOROCYCLOPENTADIONE–1,
6938	138	C6.H6.N2.O2	0–NITROANILINE
6947	138	C6.H6.N2.O2	P–NITROANILINE
9660	138	C6.H6.N2.O2	ISO–NICOTINHYDROXAMIC ACID
9665	138	C6.H6.N2.O2	2–AMINONICOTINIC ACID

MOLECULAR FORMULA SEARCH

TO SEARCH FOR A COMPLETE MF, TYPE ALL
TO SEARCH FOR A PARTIAL MF, TYPE IMBED
CR TO EXIT

USER:ALL

TYPE IN MF, (ORDER OF ATOMS: C,H,N,O,S)

USER:C6.H6.O2

FOUND 9 REFERENCES TO MF: C6.H6.O2

LIST REFERENCES, YES OR NO?

USER:YES

ID#	MW	MF	NAME
179	110	C6.H6.O2	5–METHYL–2–FURALDEHYDE
452	110	C6.H6.O2	CATECHOL
453	110	C6.H6.O2	RESORCINOL
454	110	C6.H6.O2	HYDROQUINONE
2212	110	C6.H6.O2	HYDROQUINONE
2214	110	C6.H6.O2	PYROCATECHOL
2216	110	C6.H6.O2	RESORCINOL
2217	110	C6.H6.O2	FURYL METHYL KETONE
2221	110	C6.H6.O2	2–FURYL METHYL KETONE

PEAK and MOLECULAR WEIGHT SEARCH

This search is simply a combination of two of the previously described options, the peak/intensity search and the molecular weight search. This type of search has proved useful when the molecular weight of an unknown can be found by other means, such as from chemical ionization or field ionization mass spectrometry. The molecular weight is an EXTREMELY effective "filter" in narrowing the list of possible compounds that contain a series of peaks and intensities. On the other hand, it does not allow the display of homologs having similar fragmentation patterns. An example of this is given below. In this example, a peak and intensity search by itself (not shown) gave 1031 references in the file as the answer, whereas use of the molecular weight filter led to only 2 references, both of which were of the same material.

MW AND PEAK SEARCH
(CR TO EXIT)

USER: THE MW IS: 68

USER: INTENSITY RANGE IS: 3

TYPE PEAK, INT
OR TO EXIT, 1 FOR ID,MW,MF,NAMES

USER: 41,35

FOUND 30 REFERENCES TO THAT COMBINATION

NEXT REQUEST: 28,30

FOUND 2 REFERENCES TO THAT COMBINATION

NEXT REQUEST: 1

ID#	MW	MF	NAME
1571	68	C3.H4.N2	PYRAZOLE
9138	68	C3.H4.N2	PYRAZOLE

PEAK and PARTIAL MOLECULAR FORMULA SEARCH

This is a combination of partial molecular formula and peaks/intensities, and can be used when the molecular formula is known from high resolution mass measurement or combustion analysis. It also can be used when part of the formula is found from sources such as IR or UV. (A routine to calculate all possible formula given M,M+1,M+2, etc. ions is under development.) Isotope ratios also often disclose the presence of heteroatoms and limit the number of possible formulas. This method of searching allows one to find all compounds that (a) have peaks at given m/e values and (b) contain a certain number of atom types (whose identity can be inferred, for example, from isotope patterns).

Three examples of this search are given on the next pages. In the first two examples, the searches are the same except that the first one is a qualitative partial formula search (BR) and the second is a quantitative partial formula search (BR1). The qualitative search, which allows for any number of BR atoms to be found, produced 12 references, 3 of which are BR2 compounds. The quantitative search for BR1 has only 9 references, since the BR2 answers are, of course, not included.

PEAK AND PARTIAL FORMULA SEARCH

USER: INTENSITY RANGE FACTOR IS: 3

TYPE PEAK,INT
CR TO EXIT

USER: 147,30

USER: THE NUMBER OF ATOM TYPES IS: 1

USER: GROUP 1 IS:BR

FOUND 12 REFERENCES TO THAT COMBINATION

LIST REFERENCES, YES OR NO ?

USER:YES

ID#	MW	MF	NAME
3121	176	C2.F2.CL.BR	BROMOCHLORO-1,2-DICHLOROETHYLENE
3612	224	C6.H3.CL2.BR	1-BROMO-2,5-DICHLOROBENZENE
3614	224	C6.H3.CL2.BR	1-BROMO-3,4-DICHLOROBENZENE
3784	290	C2.F2.CL2.BR2	1,2-DIFLUORO-1,2-DICHLORO-1,2-D IBROMO-METHANE
5607	224	C6.H3.CL2.BR	1,3-DICHLORO-5-BROMOBENZENE
8843	330	C16.H15.N2.O.BR	2-(ALPHA-HYDROXY-4-BROMOBENZYL) 5,6-DIMETHYLBENZIMIDAZOLE
8968	146	C3.H3.N2.BR	5-BROMOIMIDAZOLE
9354	226	C10.H11.O.BR	P-BROMOBUTYROPHENONE
10192	286	C4.H4.N2.O3.BR2	5,5-DIBROMO-6-HYDROXY-DIHYDROUR ACIL
10643	478	C27.H43.O2.BR	23R-BROMO-(25R)-5ALPHA-SPIROSTAN
10645	478	C27.H43.O2.BR	23S-BROMO-(25R)-5ALPHA-SPIROSTAN
10647	556	C27.H42.O2.BR2	23,23-DIBROMO-(25R)-5ALPHA-SPIR OSTAN

PEAK AND PARTIAL FORMULA SEARCH

USER: INTENSITY RANGE FACTOR IS: 3

TYPE PEAK, INT
CR TO EXIT

USER: 147,30

USER: THE NUMBER OF ATOM TYPES IS: 1

USER: GROUP 1 IS:BR1

FOUND 9 REFERENCES TO THAT COMBINATION

LIST REFERENCES, YES OR NO ?

USER: YES

ID#	MW	MF	NAME
3121	176	C2.F2.CL.BR	BROMOCHLORO-1,2-DICHLOROETHYLENE
3612	224	C6.H3.CL2.BR	1-BROMO-2,5-DICHLOROBENZENE
8614	224	C6.H3.CL2.BR	1-BROMO-3,4-DICHLOROBENZENE
5607	224	C6.H3.CL2.BR	1,3-DICHLORO-5-BROMOBENZENE
8843	330	C16.H15.N2.O.BR	2-(ALPHA-HYDROXY-4-BROMOBENZYL) 5,6-DIMETHYLBENZIMIDAZOLE
8968	146	C3.H3.N2.BR	5-BROMOIMIDAZOLE
9354	226	C10.H11.O.BR	P-BROMOBUTYROPHENONE
10643	478	C27.H43.O2.BR	23R-BROMO-(25R)-5ALPHA-SPIROSTAN
10645	478	C27.H43.O2.BR	23S-BROMO-(25R)-5ALPHA-SPIROSTAN

PEAK AND PARTIAL FORMULA SEARCH

USER: INTENSITY RANGE FACTOR IS: 2

TYPE PEAK, INT
CR TO EXIT

USER: 167,60

USER: THE NUMBER OF ATOM TYPES IS: 1

USER: GROUP 1 IS:C6

FOUND 3 REFERENCES TO THAT COMBINATION

LIST REFERENCES, YES OR NO ?

USER: YES

ID#	MW	MF	NAME
80	168	C6.H15.O3.B3	TRIETHYLBOROXIN
6464	168	C6.H15.O3.B3	TRIETHYLBOROXIN
6934	264	C6.H.O.CL5	PENTACHLOROPHENOL

LOSS AND MOLECULAR WEIGHT

This is another example of a combination search. In the following example the user is looking for all spectra in the file that have a large molecular ion at MW of 142 (ie. a loss of 0). (Compare these results with those from a loss and partial formula search on page 53. It is possible that a combination of MW,MF and losses/peaks would be a useful option.)

MW AND LOSS SEARCH
(CR TO EXIT)

USER: THE MW IS: 142

USER: INTENSITY RANGE FACTOR IS: 2

TYPE LOSS,INT
1 TO EXIT, 2 FOR ID,MW,MF,NAMES

USER:0,190

FOUND 23 REFERENCES TO THAT COMBINATION

NEXT REQUEST: 2

ID#	MW	MF	NAME
76	142	H8.BR.B5	BROMOPENTABORANE
2612	142	C11.H10	1-METHYLNAPHTHALENE
2615	142	C.H3.I	IODOMETHANE
2620	142	C2.H.F2.BR	BROMO-1,2-DIFLUOROETHYLENE
2624	142	C7.H7.O.CL	4-CHLORO-O-CRESOL
2627	142	C11.H10	2-METHYLNAPHTHALENE
2640	142	C7.H7.O.CL	4-CHLORO-M-CRESOL
4330	142	C11.H10	1-METHYLNAPHTHALENE
4539	142	C.H3.I	IODOMETHANE
4698	142	C11.H10	2-METHYLNAPHTHALENE
4736	142	C11.H10	1-METHYLNAPHTHALENE
4737	142	C11.H10	2-METHYLNAPHTHALENE
4833	142	C11.H10	1-METHYLNAPHTHALENE
4834	142	C11.H10	2-METHYLNAPHTHALENE
4858	142	C11.H10	2-METHYLNAPHTHALENE
5755	142	C8.H14.S	TRANS-7-THIABICYCLO(4.3.0)NONANE (TRANS-1-THIAHEXAHYDROINDANE)
5756	142	C8.H14.S	CIS-3-THIABICYCLO(4.3.0)NONANE (CIS-5-THIAHEXAHYDROINDANE)
6456	142	H8.BR.B5	BROMOPENTABORANE
7421	142	C11.H10	1-METHYLNAPHTHALENE
7422	142	C11.H10	2-METHYLNAPHTHALENE
8186	142	C7.H6.D3.N.S	1-2-D3-ETHYL-2-PYRIDTHIONE
10290	142	C11.H10	1-METHYLNAPHTHALENE
10362	142	C7.H7.O.CL	4-CHLOROMETHOXYBENZENE

LOSS AND PARTIAL MOLECULAR FORMULA SEARCH

This is still another example of a combination search. The following example indicates how one can use this option to find all compounds with 11 carbon atoms and 10 hydrogen atoms and that have a large molecular ion. Most of the answers are 1 or 2 methylnaphthalenes, although there are some others with considerably higher molecular weights.

LOSS AND PARTIAL FORMULA SEARCH

USER: INTENSITY RANGE FACTOR IS: 2

TYPE LOSS,INT
1 TO EXIT

USER:0,190

USER: THE NUMBER OF ATOM TYPES IS: 2

USER: TYPE 1 IS:C11

USER: TYPE 2 IS:H10

FOUND 22 REFERENCES TO THAT COMBINATION

LIST REFERENCES?, YES OR NO?

USER:YES

ID#	MW	MF	NAME
2612	142	C11.H10	1-METHYLNAPHTHALENE
2627	142	C11.H10	2-METHYLNAPHTHALENE
2872	158	C11.H10.O	1-METHOXYNAPHTHALENE
2873	158	C11.H10.O	2-METHOXYNAPHTHALENE
4330	142	C11.H10	1-METHYLNAPHTHALENE
4698	142	C11.H10	2-METHYLNAPHTHALENE
4736	142	C11.H10	1-METHYLNAPHTHALENE
4737	142	C11.H10	2-METHYLNAPHTHALENE
4833	142	C11.H10	1-METHYLNAPHTHALENE
4834	142	C11.H10	2-METHYLNAPHTHALENE
4858	142	C11.H10	2-METHYLNAPHTHALENE
6008	174	C11.H10.S	2-BENZYLTHIOPHENE
6766	158	C11.H10.O	2-METHYL-1-NAPHTHOL
6767	158	C11.H10.O	3-METHYL-1-NAPHTHOL
6768	158	C11.H10.O	4-METHYL-1-NAPHTHOL
7421	142	C11.H10	1-METHYLNAPHTHALENE
7422	142	C11.H10	2-METHYLNAPHTHALENE
7534	206	C11.H10.O4	2-METHYL-5-HYDROXY-7-METHOXYCHR
OMONE			
8942	174	C11.H10.S	2-BENZYLTHIOPHENE
10290	142	C11.H10	1-METHYLNAPHTHALENE
11252	206	C11.H10.O4	METHYL 5-METHYL-2,2'-BIFURAN-3'
-CARBOXYLATE			
12560	234	C11.H10.N2.O4	1,6-DIAZATETRACYCLO(4.4.3.0(3,9
).0(4,8))-TERDECA-2,5,7,10-ONE			

MOLECULAR WEIGHT and PARTIAL MOLECULAR FORMULA SEARCH

This search option allows for entering a combination of molecular weight and partial molecular formula, leading to compounds of a given molecular weight and specific atoms (e.g., 2N or O). This option can be particularly valuable where the formula of the molecular ion is known from high resolution, chemical or field ionization data. It can also be used to find all NO2 compounds with a certain molecular weight. In the example shown, the partial formula of N and S gives rise to 188 references by themselves. (N1 and S1 lead to only 140 references, (neither of these two searches are shown)). The molecular weight of 135 gives rise to 17 references by itself, while the combination program (MWMF), using 135 and N and S, reduces the answer to 2 possibilities.

MW AND MF SEARCH

USER: THE MW IS : 135

USER: THE NUMBER OF ATOM TYPES IS: 2

USER: TYPE 1 IS: N

USER: TYPE 2 IS: S

FOUND 2 REFERENCES TO THAT COMBINATION

LIST REFERENCES, YES OR NO?

USER: YES

ID#	MW	MF	NAME
322	135	C7.H5.N.S.	PHENYL ISOTHIOCYANATE
5602	135	C7.H5.N.S.	BENZOTHIAZOLE

MSDC CODE SEARCH

The MSDC codes (see Appendix D for a list of the codes or use the "LIST" option in the search system) are simply 4 digit numbers representing an arbitrary functional group classification scheme, given in Appendix D. This option accepts any MSDC code(s) and responds with the number of spectra in the file containing those code(s). The following examples indicates how this option can be used. In the first example the user wants an iodoamine and found 2 references. In the second request, the user is looking for a pyridine lactone derivative and finds 3 references to that class in the file of 12,769 spectra.

Statistics on the MSDC Codes in the file of 12,769 spectra with more than 1000 occurrances

MSDC Code	# REFS
1000	6580
1050	3916
1130	2053
1030	1725
1180	1651
1010	1504
1090	1403
1140	1240
1400	1240
1210	1180
1100	1103

MSDC CODE SEARCH

TYPE CODE, CR TO EXIT, 1 FOR ID,MW,MF AND NAME

USER:1290

# REFS	CODES
770	1290

NEXT REQUEST: 1420

# REFS	CODES
2	1290 1420

NEXT REQUEST: 1

ID#	MW	MF	NAME
11417	279	C7.H6.N.O3.I	3–AMINO–5–IODO–SALICYCLIC ACID
11418	293	C8.H8.N.O3.I	METHYL 3–AMINO–5–IODO–SALICYLATE

MSDC CODE SEARCH

TYPE CODE, CR TO EXIT, 1 FOR ID,MW,MF AND NAME

USER:1240

# REFS	CODES
177	1240

NEXT REQUEST: 1070

# REFS	CODES
34	1240 1070

NEXT REQUEST: 1090

# REFS	CODES
3	1240 1070 1090

NEXT REQUEST: 1

ID#	MW	MF	NAME
8276	221	C14.H7.N.02	1–CARBOXY–10–HYDROXY–PHENANTHRIDINE LAC
TONE			
12511	223	C14.H9.N.02	2–PHENYL–3, 1–BENOXAZINE–4–ONE
12514	301	C14.H8.N.02.BR	2–(4'–BROMOPHENYL)–4H–3, 1–BENZOXAZIN–4–
ONE			

NSDC CODE AND MOLECULAR WEIGHT SEARCH

Another combination search option. The two example given on the next pages show how a given class or type of compound can be readily found. The first example shows that by requesting an aromatic compound with a MW of 78, the 7 benzene spectra in the file are found. The second request gives all the aldehydes in the file that have a MW of 98.

```
MW AND CODE SEARCH
CR TO EXIT

USER:  THE MW IS :78


TYPE CODE
CR TO EXIT, 1 FOR ID,MW,MF,NAMES

USER:1050

FOUND       7 REFERENCES TO THAT COMBINATION

NEXT REQUEST:  1

  ID#          MW          MF                          NAME

 1994          78  C6.H6                       BENZENE
 4018          78  C6.H6                       BENZENE
 4093          78  C6.H6                       BENZENE
 4147          78  C6.H6                       BENZENE
 4260          78  C6.H6                       BENZENE
 5434          78  C6.H6                       BENZENE
 5455          78  C6.H6                       BENZENE
```

MW AND CODE SEARCH
CR TO EXIT

USER: THE MW IS:98

TYPE CODE
CR TO EXIT, 1 FOR ID,MW,MF,NAMES

USER:1170

FOUND 6 REFERENCES TO THAT COMBINATION

NEXT REQUEST: 1

ID#	MW	MF	NAME
775	98	C6.H10.O	2–METHYL–2–PENTENAL–1
893	98	C6.H10.O	2–HEXENAL
2106	98	C6.H10.O	2–METHYL–2–PENTENAL
7113	98	C6.H10.O	ISOHEXENAL
8591	98	C6.H10.O	2–METHYL–PENT–2–EN–1–AL
8595	98	C6.H10.O	CYCLOPENTANE–CARBALDEHYDE

MSDC CODE AND PARTIAL MOLECULAR FORMULA SEARCH

Yet another combination search option. The example given below is designed to find all nitro compounds that have 6 carbon and 6 hydrogen atoms as well as a second nitrogen (a total of 2) that need not be a nitro nitrogen.

CODE AND PARTIAL FORMULA SEARCH

TYPE CODE
CR TO EXIT

USER: 1310

USER: THE NUMBER OF TYPES WILL BE: 3

USER: GROUP 1 IS:C6

USER: GROUP 2 IS:H6

USER: GROUP 3 IS:N2

FOUND 2 REFERENCES TO THAT COMBINATION

LIST REFERENCES, YES OR NO?

USER: YES

ID#	MW	MF	NAME
6938	138	C6.H6.N2.O2	O–NITROANILINE
6947	138	C6.H6.N2.O2	P–NITROANILINE

MSDC CODE AND PEAK SEARCH

This is another of the combination search options. The following example shows how one can search for lactones and need only to use one peak to narrow the file down from 12,769 spectra to 14 references.

PEAK AND CODE SEARCH

TYPE CODE
CR TO EXIT

USER: 1240

USER: INTENSITY RANGE IS: 3

TYPE PEAK,INT
CR TO EXIT, 1 FOR ID,MW,MF,NAMES

USER: 85,100

FOUND 14 REFERENCES TO THAT COMBINATION

NEXT REQUEST: 1

ID#	MW	MF	NAME
550	184	C11.H20.O2	GAMMA UNDECALACTONE
1643	100	C5.H8.O2	GAMMA VALEROLACTONE
1644	114	C6.H10.O2	GAMMA-CAPROLACTONE
1651	128	C7.H12.O2	GAMMA-HEPTALACTONE
1658	142	C8.H14.O2	GAMMA-OCTALACTONE
1668	156	C9.H16.O2	GAMMA-NONALACTONE
1671	170	C10.H18.O2	GAMMA-DECALACTONE
1680	184	C11.H20.O2	GAMMA-UNDECALACTONE
1688	254	C16.H30.O2	GAMMA-PALMITOLACTONE
1689	282	C18.H34.O2	GAMMA-STEAROLACTONE
2119	100	C5.H8.O2	HYDROXY VALERIC ACID LACTONE
7708	246	C15,H18,O3	6-EPI-ALPHA-SANTONIN
10758	216	C9,H12,O6	1,2-ISOPROPYLIDENE-ALPHA-D-GLUC OFURANURONO-6,3-LACTONE
11858	282	C12.H20.O6.B2	TARTARIC ACID N-BUTYL BORONATE

MSDC CODE AND LOSS SEARCH

This is another of the numerous combination search options. Here, in the example below, the user is looking for amides that lose 16 and 43 from the molecular ion. Including duplicates, 14 spectra are found with only two peaks entered.

LOSS AND CODE SEARCH

TYPE CODE
CR TO EXIT

USER: 1260

USER: INTENSITY RANGE FACTOR IS: 4

TYPE LOSS, INT
2 TO EXIT, 1 FOR ID,MW,MF,NAMES

USER: -43,30

FOUND 93 REFERENCES TO THAT COMBINATION

NEXT REQUEST: -16,20

FOUND 14 REFERENCES TO THAT COMBINATION

NEXT REQUEST: 1

ID#	MW	MF	NAME
167	59	C2.H5.N.O	ACETAMIDE
285	87	C4.H9.N.O	BUTYRAMIDE
1255	71	C3.H5.N.O	ACRYLAMIDE
7503	97	C5.H7.N.O	3-AMIDOCYCLOBUTENE
8759	60	C.H4.N2.O	UREA
9057	60	C.H4.N2.O	UREA
9058	74	C2.H6.N2.O	N-METHYLUREA
9059	88	C3.H8.N2.O	N,N-DIMETHYLUREA
9674	136	C7.H8.N2.O	3-AMINOBENZAMIDE
9769	87	C4.H9.N.O	ISO-BUTYRAMIDE
9964	215	C14.H17.N.O	2-(1-CYCLOHEXENYL) METHYLBENZAMIDE
10828	87	C4.H9.N.O	N-BUTYRAMIDE
10829	87	C4.H9.N.O	ISOBUTYRAMIDE
12488	128	C4.H4.N2.O.S	ISOTHIRZOLE-3-CARBOXAMIDE

COMPLETE SPECTRUM SEARCH

The conversion of the Biemann search system (that EPA has operational at Battelle) into this system is currently being undertaken (14). Details for using the option when available can be obtained from John McGuire or Steve Heller. The summer of 1974 is the planned date for the PDP-10 version of the Biemann/Battelle software to be operational.

It will also be made available on the GE MARK III Timesharing System as well as to any interested parties on a no-profit basis.

Other complete spectrum search systems are also being studied for possible future options in the system. One such program is the McLafferty STIRS program(15). Users interested in this, or other programs should make their views known via the CRAB option or other means.

DISSIMILARITY INDEX

The Dissimilarity Index (DI) option allows one to compare spectra quantitatively either within the file or between the file and unknown.

The index uses the differences in the squares of the intensities at every mass from 12 to 400 and further emphasizes differences when there is a peak in one spectrum, but none in the other. (This extra emphasis was done to accentuate differences or dissimilarities heavily and does distort results in some cases). In the case where there is a peak in one spectrum but not in the other, difference in the squares of the intensities are used, rather than the square root of the difference in the squares. $(D_f^2 - D_d^2$, but since $D_d = 0$, the contribution is D^2 rather than $D = \sqrt{D_f^2}$. See the equation on page 71.) This has the effect of providing, in general, reasonable separation for low molecular weight compounds and much greater separation for high molecular weight compounds. The method leads to great dissimilarity of non-homologous compounds because many peaks will be absent in one spectrum that are present in the other. It is felt that the search itself provides a sufficient degree of information regarding homologous compounds so that this

index can be used to reflect other information. It has also been found that the empirically derived DI effectively separates isomers, terpenes, halogen-containing compounds from mass spectra of similar compounds and is most valuable in this laboratory in checking supposed "duplicate" spectra in file.

An arbitrary normalization constant of 400 is used to scale the INDEX numbers down to a range of 0 to about 50 and originated from the mass range being used. The upper value of DI is approximate due to the arbitrary nature of the scaling factor. In addition to the 12-400 mass range, the user has the option of changing the range to any range between m/e 1 and m/e 500 he wishes to examine.

Two examples of this option are given on the following pages. The first example uses the answers found from the sample amide search presented in the MSDC Code and loss search example on page 67. In the second example, one of the resorcinols found from the complete MF search (page 43) is used as the standard and a number of answers from that search are compared with it.

Neither of these example includes what happens when you type "MINE" or "PREV". If you choose MINE, the computer will than ask you to type the COMPLETE spectrum into the computer. If you have done this already on a previous

occasion and have saved the file on your disk area, then you can choose the PREV option. Plans are underway to be able to have various minicomputers "talk" directly to the PDP-10 and GE central computer. Also the ability to transmit paper tape directly into the computer via the terminal is being developed.

$$DI = \sqrt{\sum_{N=12}^{400} \left| I_1(N) - I_2(N) \right|^K} \Big/ 400$$

K = 2 if and only if I_1 or I_2 = 0, else K = 1

SPECTRUM DISSIMILARITY COMPARISON
(ANSWERS RANGE FROM 0.0 TO 50.0)

USE 12--400 MASS RANGE (REG) OR OTHER(MINE)

USER:REG

USER UNKNOWN (MINE), PREVIOUS UNKNOWN (PREV)
OR FILE SPECTRUM (FILE)?

USER: FILE

FILE SPECTRUM ID # PLEASE

USER: 2216

USER: THE # OF SPECTRA FOR COMPARISON ARE: 7

USER: ID # 1 IS: 179

USER: ID # 2 IS: 452

USER: ID # 3 IS: 453

USER: ID # 4 IS: 454

USER: ID # 5 IS: 2212

USER: ID # 6 IS: 2214

USER: ID # 7 IS: 2221

STD: 2216

ID#	DISSIMILARITY
179	0.34
452	0.17
453	0.14
454	0.14
2212	2.46
2214	25.00
2221	0.61

SPECTRUM DISSIMILARITY COMPARISON
(ANSWERS RANGE FROM 0.0 TO 50.0)

USE 12-400 MASS RANGE (REG) OR OTHER(MINE)

USER:REG

USER UNKNOWN (MINE), PREVIOUS UNKNOWN (PREV)
OR FILE SPECTRUM (FILE)?

USER: FILE

FILE SPECTRUM ID # PLEASE

USER: 285

USER: THE # OF SPECTRA FOR COMPARISON ARE: 4

USER: ID # 1 IS: 267

USER: ID # 2 IS: 9769

USER: ID # 3 IS: 10828

USER: ID # 4 IS: 10829

STD: 285

ID#	DISSIMILARITY
267	1.25
9769	3.63
10828	1.00
10829	2.67

SUBSTRUCTURE SEARCH

The substructure search (SSS) option is available, but not yet with the mass spec data base(16). This is option 2 of the DCRT/CIS and a manual for its use is available from Richard J. Feldmann, Bldg. 12A, Rm. 3001, DCRT, NIH, Bethesda, Maryland 20014 USA (301-496-1100).

When the SSS is interfaced with the mass spec file it is anticipated that the SSS manual will be incorporated into this manual.

The Chemical Abstracts Service(CAS) registry numbers (REGN) are being obtained for the data base as both a unique indentification number and as a link to the SSS.

MASS SPECTRAL SPECTRUM PRINTOUT

Once you have obtained an ID# from any of the previous searches, you may have the full spectrum (NOT just the three largest peaks in every 14 m/e) typed out. The spectrum retrieval program requires the ID#. The ID# is completely arbitrary and most likely will change every time the data base is updated. After giving the ID#, the program responds with the number of peaks in the spectrum. If there are more than you care to have typed out after requesting a type out, you can limit the amount typed out by specifying a lower and an upper limit to the m/e of the spectrum peaks. Lastly you can specify that you want to look at peaks with a minimum intensity level. Remember the intensity level goes from 0 to 100 (0.1-100.0%). This new option now also contains information about the source of the spectrum.

The source information printed out is in a compressed form. The details of the format is given in Appendix E. The first line contains the collection code letter (NSC,API,DOW, etc.) and the collection number, followed by the contributors' name &/or institution. The next line contains information about the instrument, inlet type (gas, direct, etc.), then the inlet temperature, source temperature and ionizing energy (all 1I3 format, ie. 3

spaces), then the ion accelerating voltage (4 characters, 1A4) and lastly, the pressure in torr (eg. 1.7 x 10-5 is 17-5). Not all the source information is available.

Three examples are given on the next pages. In the first, HBr, the entire spectrum is typed out. In the next section on display and plotting of spectra, these same data were used to produce the display and plot of HBr on page 83. LSD is the second example, and in this case, only those peaks with an intensity greater than or equal to 5% are printed out. The symbol ">" is meant to mean "greater than or equal to", not "greater than" in this system because the proper symbol is not available on terminals in general.) In the next section (page 84), the entire LSD spectrum is plotted out , not just the peaks with intensity > 5%. Lastly, a spectrum of an aspartic acid derivative is typed out and is also plotted and can be seen on page 85.

ID# FOR FULL SPECTRUM
CR TO EXIT

USER: 57

ID#	MW	MF	NAME
57	80	H.BR	HYDROGEN BROMIDE

SOURCE INFO:

AST L9CALLERY CHEMICAL CO., CALLERY, PENNSYLVANIA

CEC21-103B 30270 0 0

THERE ARE 7 PEAKS IN SPECTRUM # 57 , LIST ?, YES OR NO ?

USER: YES

USER: THE MIN & MAX M/E ARE: 0,100

USER: TYPE ALL M/E'S WITH INTENSITY >0

M/E	INT
2	1
40	3
41	3
79	45
80	100
81	44
82	98

ID# FOR FULL SPECTRUM
CR TO EXIT

USER: 9339

ID#	MW	MF	NAME
9339	323	C20.H25.N3.O	LYSERGIC ACID DIETHYLAMIDE

SOURCE INFO:

MSC02567S.W.BELLMAN FOOD AND DRUG ADMIN., BROOKLYN, N.Y., USA

AEI MS12 DIRECT 0175 70 0

THERE ARE 64 PEAKS IN SPECTRUM # 9339, LIST ?, YES OR NO ?

USER: YES

USER: THE MIN & MAX M/E ARE: 0,500

USER: TYPE ALL M/E'S WITH INTENSITY > 5

M/E	INT
27	5
29	25
41	5
42	14
43	7
44	11
55	5
57	7
58	5
72	17
100	8
111	9
127	5
128	11
151	6
152	8
153	6
154	13
167	14
178	8
179	9
180	17
181	41
182	8
192	10
193	5
195	5
196	17
205	10
206	7
207	29
208	13
220	9
221	64
222	36
223	32
224	6
280	5
323	100
324	21

ID# FOR FULL SPECTRUM
CR TO EXIT

USER: 12404

ID#	MW	MF	NAME
12404	349	C13.H31.N.O4.SI3	N,O,O'-TRI-TMS-ASPARTIC ACID

SOURCE INFO:

MSC 5835K. BERGSTROM KAROLINSKA INST., STOCKHOLM, SWEDEN

LKB 9000 0 0 70 0

THERE ARE 18 PEAKS IN SPECTRUM #12404 , LIST ? YES OR NO ?

USER: YES

USER: THE MIN & MAX M/E ARE: 0,400

USER: TYPE ALL M/E'S WITH INTENSITY > 0

M/E	INT
45	5
59	3
73	42
75	10
93	13
100	12
117	6
130	6
147	13
160	13
188	5
202	8
218	17
232	100
244	5
306	4
334	5
349	2

SPECTRUM DISPLAY AND PLOTTING OPTION

In addition to the spectrum printout option that will work on any teletype, those users with graphics terminals can obtain a graphic bar plot of a spectrum. Those users on the PDP-10 can also obtain CALCOMP or ZETA plots of their spectra. On the PDP-10 a number of graphics terminals can be used. On the GE MARK III Foreground Timesharing system, only a Tektronix 4000 series terminal can be used. At present the following graphics terminals work with the PDP-10:

1. DEC-340
2. DEC-GT-40
3. Tektronix 4000 Series
4. Computek
5. Ards
6. Adage AGT-30

Most of the graphics package on the PDP-10 was written by R. Sproull and K. Stevens. The PDP-10 also allows for the image on the display terminal to be put onto a *.PLX disk file, for plotting on a CALCOMP or ZETA plotter, using

the PLOTX package on the PDP-10. (Written by R. Sproull). Both the PDP-10 and GE plotting first give the entire spectrum and then allow you to choose any 100 amu interval for expansion. For example:

```
USER RESPONSE: PLOT

THIS ROUTINE REQUIRES A DISPLAY TERMINAL -
OTHERWISE A HUGE VOLUME OF GARBAGE WILL SPEW FORTH

ID# FOR DISPLAY, CR TO EXIT

USER: 57

WHICH DISPLAY TERMINAL ARE YOU USING ?

0 FOR DEC-340     2 FOR ADAGE
4 FOR TEKTRONIX   5 FOR GT-40

USER: 4

PLOT THIS SPECTRUM ?  YES or NO ?

USER: YES                    (see page 83)

DIFFERENT STARTING POINT ?, YES OR NO ?

USER: NO

ID# FOR DISPLAY, CR TO EXIT

USER: 9108

PLOT THIS SPECTRUM ?, YES OR NO ?

USER: YES                    (see page 86)

DIFFERENT STARTING POINT ?, YES OR NO ?

USER: YES

NEW STARTING POINT IS: 25

PLOT THIS SPECTRUM ?, YES OR NO ?
```

USER: YES (see page 87)

DIFFERENT STARTING POINT ?, YES OR NO ?

USER: YES

NEW STARTING POINT IS: 140

PLOT THIS SPECTRUM ?, YES OR NO ?

USER: YES (see page 88)

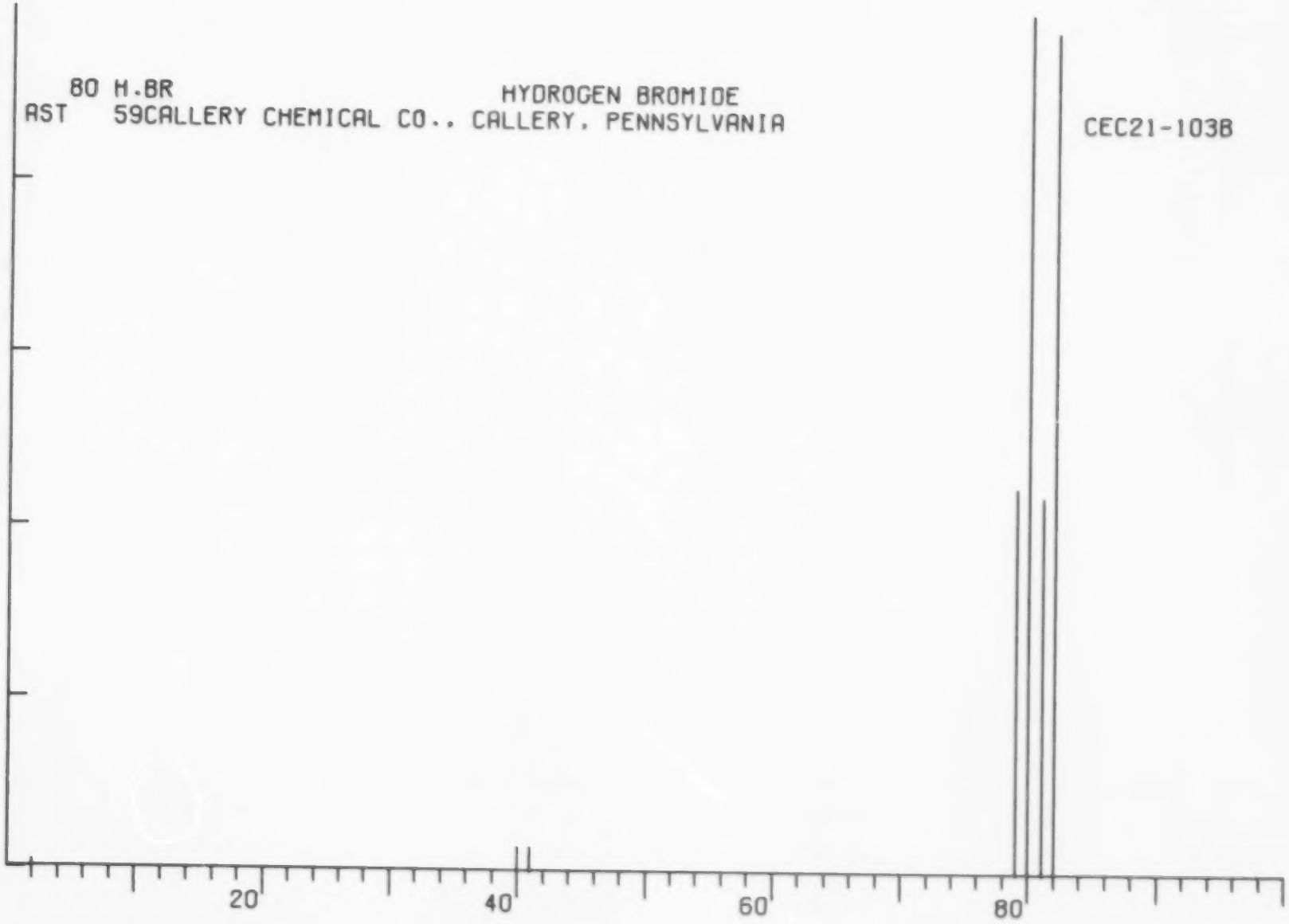
DIFFERENT STARTING POINT ?, YES OR NO ?

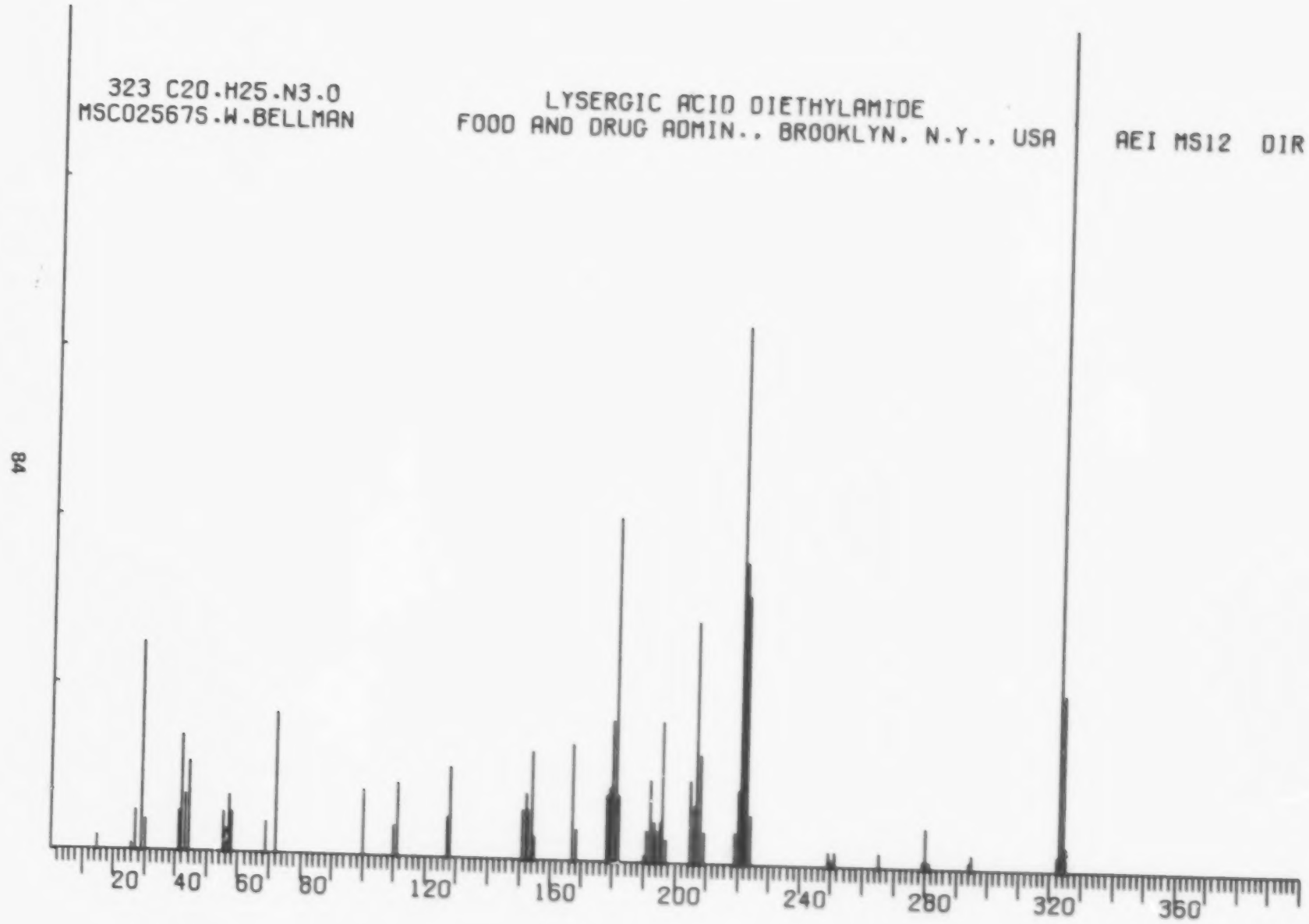
USER: NO

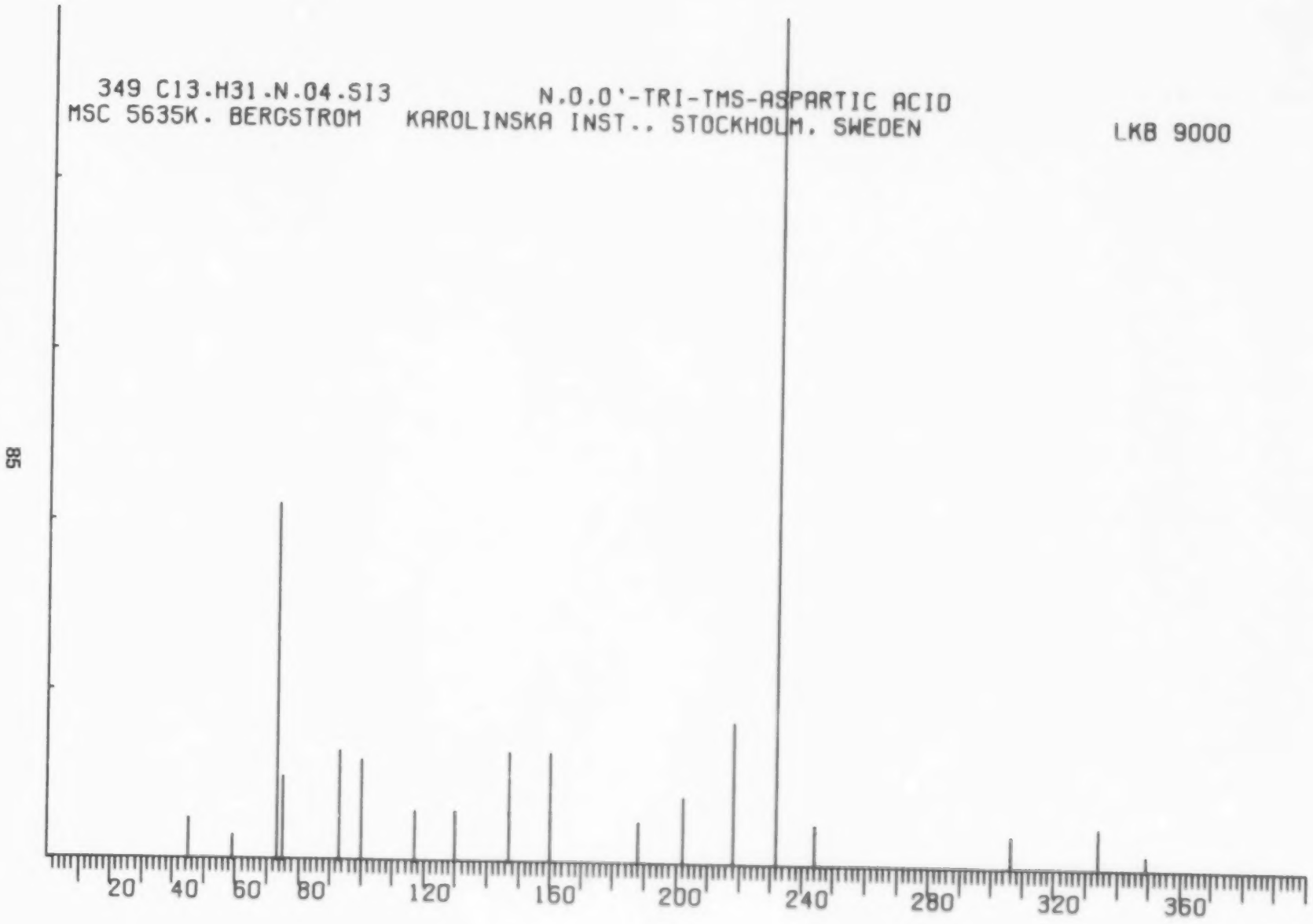
ID# FOR DISPLAY, CR TO EXIT

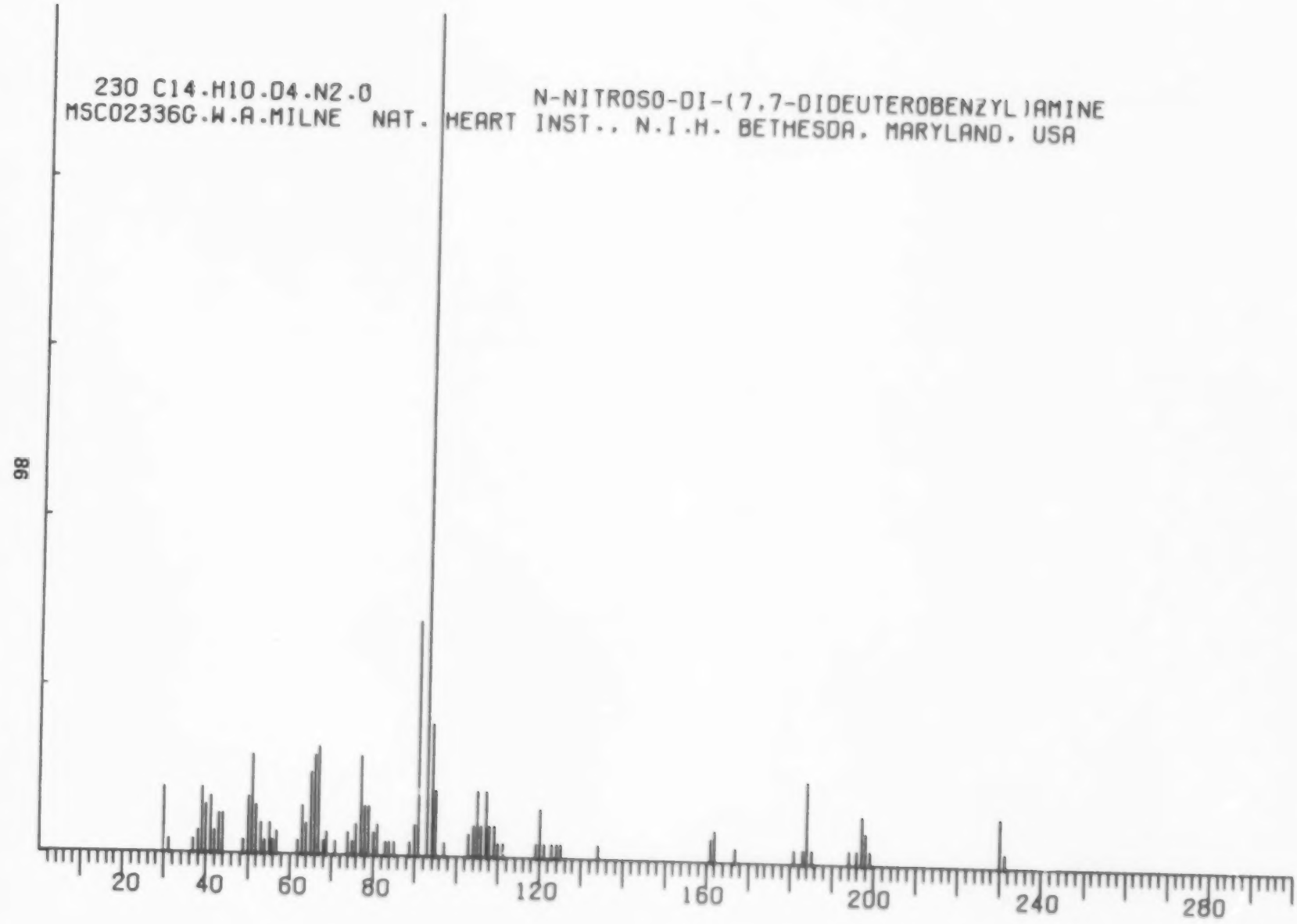
USER:_(CR)

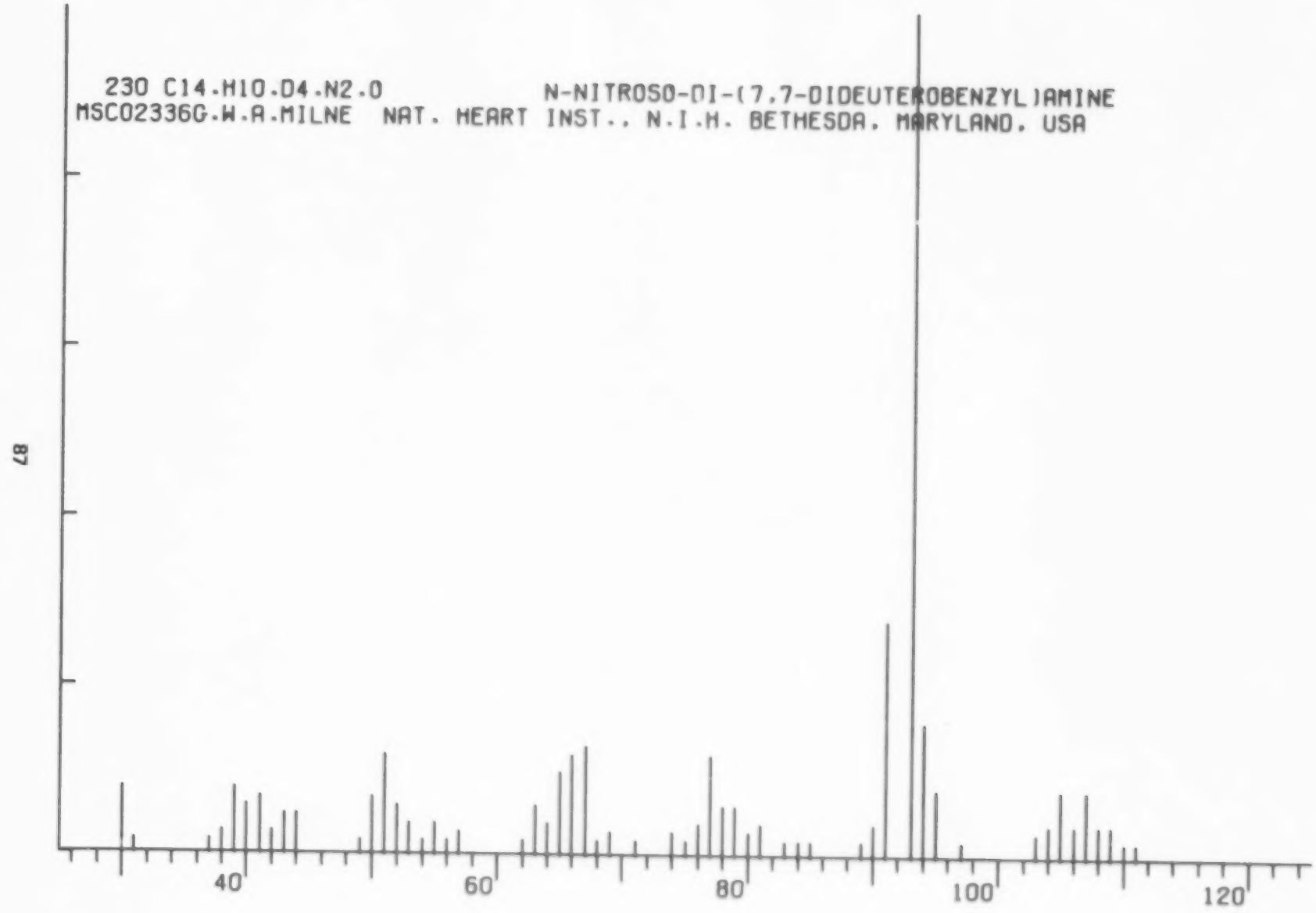
The following pages are examples of the PLOT option. The first spectrum displayed is always the entire spectrum. If you want to look at only a region or section of the spectrum, the program will accept a different starting point (as the dialog above indicates). The partial spectrum is then displayed from the starting point to 100 amu above the starting point. That is, the partial spectrum is always 100 amu wide, beginning at any amu you choose (eg. 100 or 145 or 222 or ...). The last example (pages 86 - 88) is a series of plots of ID# 9108 The first is the complete plot with a scale of 0-300 m/e. In the second the scale is from m/e 25 - 125. The last plot is from m/e 140 to 240.

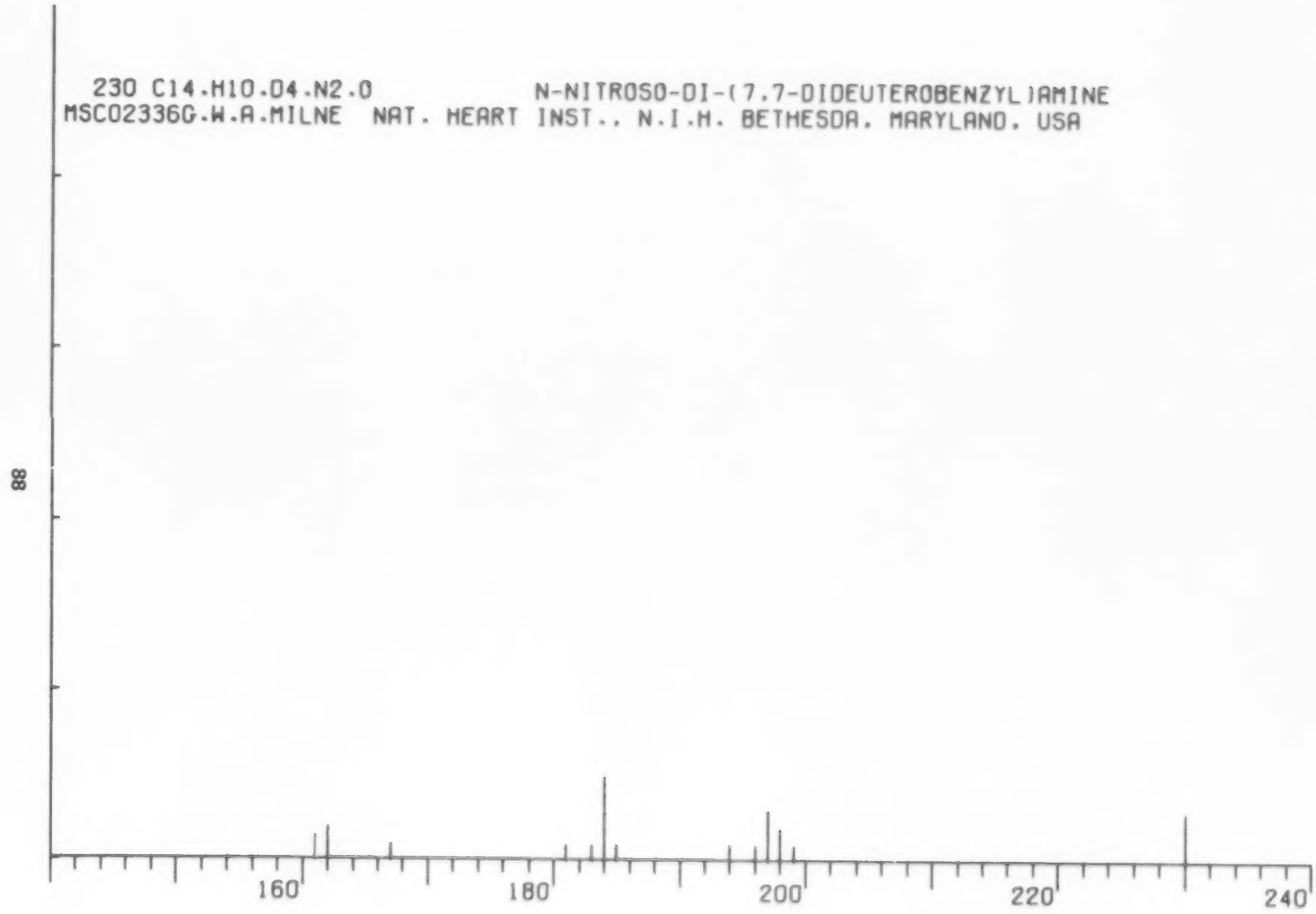

80 H.BR
HYDROGEN BROMIDE
AST 59CALLERY CHEMICAL CO., CALLERY, PENNSYLVANIA
CEC21-103B
20
40
60
80


323 C20.H25.N3.O
MSC02567S.W.BELLMAN
LYSERGIC ACID DIETHYLAMIDE
FOOD AND DRUG ADMIN., BROOKLYN, N.Y., USA
AEI MS12 DIR
84
20
40
60
80
120
160
200
240
280
320
360


349 C13.H31.N.04.SI3
N.O.O'-TRI-TMS-ASPARTIC ACID
MSC 5635K. BERGSTROM
KAROLINSKA INST., STOCKHOLM, SWEDEN
LKB 9000
85
20
40
60
80
120
160
200
240
280
320
360


230 C14.H10.D4.N2.0
MSC02336G.W.A.MILNE NAT. HEART INST., N.I.H. BETHESDA, MARYLAND, USA
N-NITROSO-DI-(7,7-DIDEUTEROBENZYL)AMINE
86
20
40
60
80
120
160
200
240
280


230 C14.H10.D4.N2.O
N-NITROSO-DI-(7,7-DIDEUTEROBENZYL)AMINE
MSC02336G.W.A.MILNE NAT. HEART INST., N.I.H. BETHESDA, MARYLAND, USA
87
40
60
80
100
120


230 C14.H10.D4.N2.0 N-NITROSO-DI-(7,7-DIDEUTEROBENZYL)AMINE
MSC02336G.W.A.MILNE NAT. HEART INST., N.I.H. BETHESDA, MARYLAND, USA
88
160
180
200
220
240

MICROFICHE DISPLAY

For those who have manual or computer driven microfiche viewers this is a another alternative for spectral display. The microfiche generated are 42X microfiche. The computer driven unit that this system works with is a COMCARD viewer from Image Systems, Culver City, California. The cost of producing the microfiche masters is quite high, and there are copyrights on the data. Inquiries about microfiche should be made to: Steve Heller (US government, PDP-10 users), MSDC Staff (all others using the GE network). The microfiche option requires an ID# as input. N.B. Since the ID# are arbitrary and change as the data base is updated, the microfiche can become obsolete and fairly useless rather quickly. In the use of the manual viewers, the fiche number and matrix position on that fiche are typed out enabling the user to get the fiche and put it in the viewer. With the COMCARD, after the ID# is typed in, the unit performs the task of finding the proper fiche and frame displays it on the screen in less than four seconds. For example:

USER RESPONSE: FICHE

MANUAL(M) OR COMPUTER(C) FICHE LOOKUP ?, M OR C ?

USER: M

ID# FOR FICHE AND POSITION,CR TO EXIT

USER: 100

FICHE #: 1 FRAME: D9

ID# FOR FICHE AND POSITION,CR TO EXIT

USER: __ (CR)

MANUAL(M) OR COMPUTER(C) FICHE LOOKUP ?, M OR C ?

USER: C

THIS ROUTINE DRIVES THE IMAGE SYSTEMS
MICROFICHE VIEWER ONLY !!

ID# FOR VIEW, CR TO EXIT

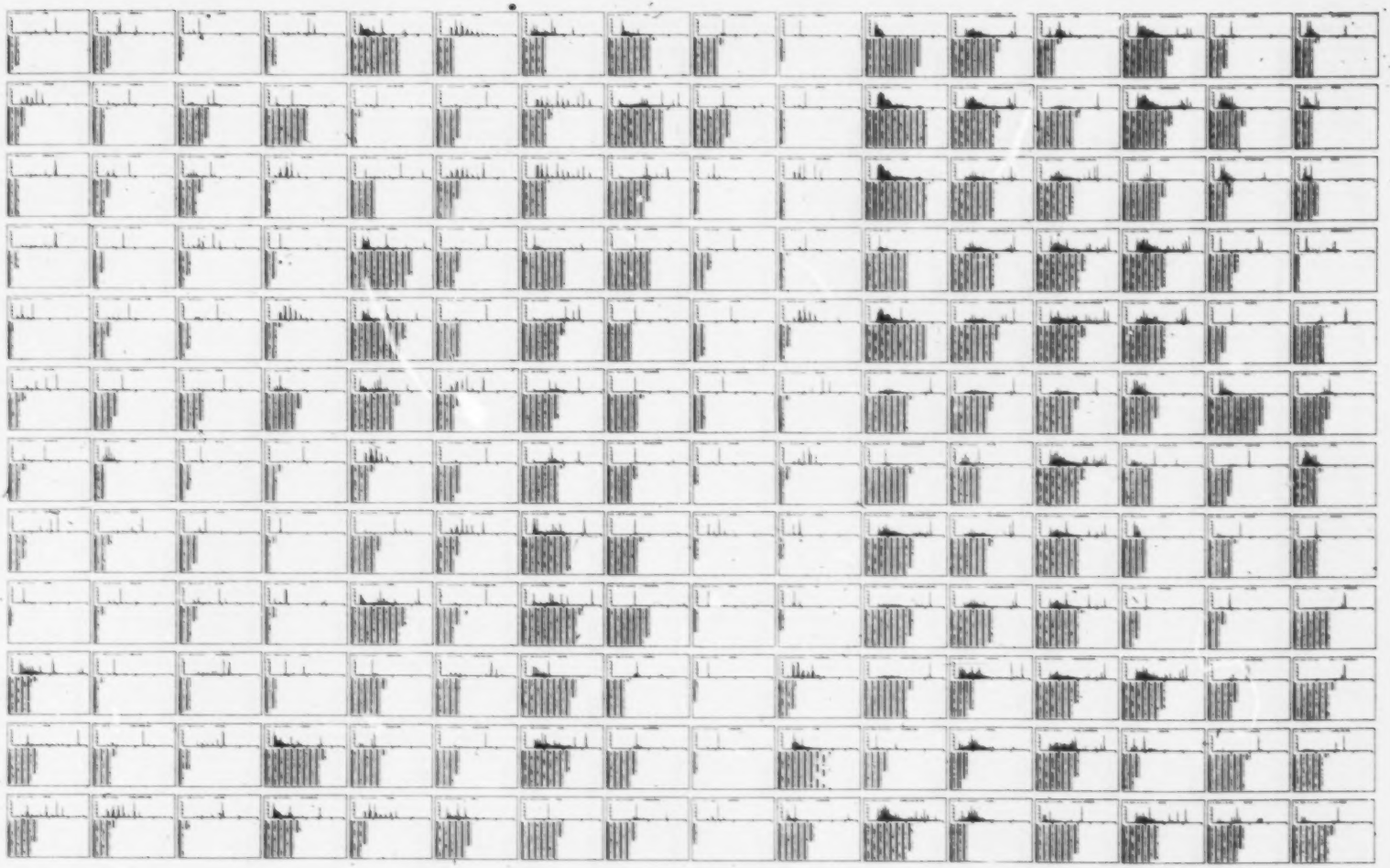
USER: 100

(The viewer is then driven to the necessary position to put spectrum #100 on the viewer screen.)

The next page has a picture of the COMCARD unit, with the user holding a microfiche in his hand. The page following that is a blow-up of a typical microfiche.

G UNITS

MASS SPECTRA 193- 384



CRAB: COMMENTS/COMPLAINTS

To facilitate feedback and suggestions, the CRAB option has been written. The program starts by requesting your name, address company and message. All information entered is free form, so type away. When you are finished type ZZZ and a carriage return (CR) and your message will be duly delivered. Suggestions for new search options, questions on the system, complaints on the running of the program, comments on errors in the data, etc. are all examples of what is hoped for. The burden of finding errors, bad data, duplicate entries, etc. must fall on the users of the search system. Errors should be as fully documented as possible. It is hoped that the file will be dynamic and bad data corrected or removed at reasonable intervals. However, no changes or improvements will occur unless YOU, the user, help.

Please feel free to use this often. There are humans connected to the other end and we would like to hear from you, even if just to chat.

All CRABS will be acknowledged.

PLEASE TYPE YOUR NAME AND ADDRESS AND COMMENT.
WHEN YOU ARE DONE, TYPE ZZZ AND CARRIAGE RETURN. TO
CONTINUE THE MASS SPEC SEARCH YOU MUST TYPE CHEM AGAIN.

JOHN DOE, CHEMICAL CORP. OF AMERICA, PO BOX 1973, NEW YORK,
NEW YORK

WHEN ARE YOU GOING TO ADD THE MSDC BULLETIN TO THE SYSTEM??

ZZZ

EXIT

ENTERING DATA

In addition to improving the quality of the file and the system with CRAB, it is necessary to increase the size of the file. One way to do this in a manner as painless as possible is to use the HARVEST option. Another way to add to the file is to send spectra to anyone listed in Appendix B. The MSSS file format is given in Appendix E. However if you do not or can not get your data in computer readable form and want to add your data to the file, please send it on data collection sheets available from Hank Fales, Bill Milne, John McGuire or Steve Heller. These data sheets require essentially the same information as the HARVEST program.

The HARVEST option is initiated by typing "DATA" as your option choice. Once initiated, the program first requests your name and address (3 lines). It then requests the name of the compound you wish to enter. Please try to use the Chem Abstracts name in addition to any trivial or common name you have. Then you enter the Chem Abstract Registry Number (REGN), otherwise just a carriage return. The REGN can be usually found rather painlessly by looking up the name in the CA Subject Index (starting with Volume 71 or the 8th Collective Index). It can also be found in the

Formula Index to CA using the molecular formula and the name. Next you enter the Wiswesser Line Notation (WLN), if known. Otherwise just hit a carriage return (CR). Entering the REGN and/or WLN will greatly aid in implementation of a structure searching option. The next item is the molecular formula. The format for this is C,H,N,O,S, the halogens (F,Cl,Br,I) and then alphabetical. Polymers have a MF of 9999. Put a period between each atom type, but no period at the end. In the case of only one of an element, omit the 1 (eg. C.H4 and not C.H4. or C1.H4). Next comes the molecular weight, as an integer please. (Assume CL is 35 because that is the way you search for it in the search program and a polymer is arbitrarily 9999). Next enter the MSDC classification codes that apply to the compound. You must enter the codes or the program will not continue on! The codes are all integers and should be separated by a space or a comma. A list of the codes can be obtained by using the "LIST" option. A list of the codes is also in this manual (see page 112). Then the program begins to request the following list of information, one item at a time:

1. Instrument
2. Inlet System
3. Inlet Temperature (C)
4. Source Temperature (C)
5. Electron Voltage (eV)

6. Ion Accelerating Voltage (V)

7. Pressure (Torr or mm Hg)

Last, but not least, the peaks and their intensities are entered, one at a time, first the mass and then the intensity followed by a carriage return (CR). The mass/peak and intensity must be separated by a space or comma. The peaks and intensities must be integers. The intensity range of 0.1% to 100.0% is rounded off for the program to 0% to 100%, however you can put the intensities in either way. However, remember there must be a base peak (Intensity=100) in the data, or the program will complain and start to request the peaks and intensities again. Also the peaks and intensities must be entered in ascending order, and no peak value can be duplicated. If either occurs, the program complains and backs up one peak and allows you to continue. Remember the peak and the intensity must be separated by a space or a comma. After the last peak is entered, just hit the carriage return(CR) and the program will respond with the number of peaks entered and ask if you wish to enter more data or exit. An example is given on the following page.

BE NOT DECIVED, GOD IS NOT MOCKED
FOR WHATEVER A MAN SOWETH, THAT SHALL HE ALSO REAP.

MY NAME IS: L. E. HARRIS
MY ADDRESS (LINE 1 OF 3) IS: U.S. EPA, AWC LAB
ADDRESS LINE 2 IS: 1014 BDWY
ADDRESS LINE 3 IS: CINCINNATI, OHIO 45202 USA
THE NAME FOR THE COMPOUND IS: CAPROLACTAM
THE CA REGN IS: 105602
THE WLN IS: T7MVTJ
THE MOLECULAR FORMULA IS: C6.H11.N.0
THE MOLECULAR WEIGHT IS: 113
THE MSDC CODES ARE: 1030, 1270
RECORDING INSTRUMENT WAS: FINNIGAN
INLET SYSTEM: GC
INLET TEMP (C): 120
SOURCE TEMP (C): APPROX. 150
ELEC. VOLTAGE (EV): 70
ION ACCELERATING VOLTAGE (KV): 3
PRESSURE (TORR): 10-5

NOW GIVE PEAKS AND INTENSITIES

EACH LINE SHOULD CONTAIN ONE PEAK FOLLOWED BY
A COMMA AND THEN THE INTENSITY

THE PEAKS SHOULD BE IN SEQUENCE
THE INTENSITIES SHOULD BE BETWEEN 0 AND 100

GIVE A CARRIAGE RETURN TO FINISH INPUTTING PEAKS.

39	12
41	18
42	27
43	8
44	7
50	1
51	2
52	3
53	5
54	6
55	82
56	67
57	7
67	11
68	6
69	4
70	2
79	2
80	2
84	52
85	70
86	3
98	1
111	2
112	4
113	100
114	7

THERE WERE 28 PEAKS IN YOUR SPECTRUM

PROGRAM: DO YOU WANT TO ENTER ANOTHER SPECTRUM YES/NO

USER:NO

EXIT

NEWS

The NEWS option is our way of communicating with the users easily and quickly. The NEWS is updated when neccessary.

Content of the Data Base

Another problem is the content of the data base. As has been pointed out in other sections of this manual, as well as at scientific meetings and in publications dealing with the NSSS, only YOU, the user can solve the problem by submitting your spectra to the system. The file has been established from what spectra users have submitted to the system in the past and thus reflects the research interests of relatively few mass spectrometry research groups. If you find that compounds of interest to you are not in the data base - then its primarily up to you to fix the situation by submitting your spectra.

The original file of 8124 and 8782 spectra were obtained with the aid of MIT, NIH, Baylor and EPA. The new and current file of 12,769 is a new file and the complete file from the MSDC. A large number of duplicates and incompletely documented spectra from the recently used 8782 spectra file data base are NOT in the new 12,769 spectra data base. Work is underway to provide more qualitative and quantitative descriptions of the file. The MSDC codes are one qualitative method of describing the compounds in the file. The CAS REGN, when obtained, will finally

quantitatively define the number of different compounds in the file. This number will obviously be less than the number of spectra in the file owing to duplicates, etc.

The current file of 12,769 spectra contain the following collections:

1. ASTM E14 Uncertified Spectra
2. Dow Chemical Co. Spectra
3. API Standard Spectra
4. TRC Spectra
5. MSDC Spectra Collection

The data base is expected to be expanded and updated again in the summer of 1974 when the approximately 24,000 spectra John Wiley Registry Data Base, compiled by Stenhagen, Abrahamsson and McLafferty will be merged into the current data base. Again let it be made perfectly clear, the frequency of the updates is dependent on the user contributing to the system. The system, if it is to be of value, must be a worldwide effort of the mass sepctrometry community.

Comments

While many users can and will submit spectra for inclusion in tha data base, it is realized that there are proprietary files that cannot be made public. The GE Mark III Service now has an option that will allow one to search his own private file stored on his own secure disk account area using the same search programs that search the public files. Users interested in details regarding costs and other related matters should use the CRAB message or contact their local Mark III Timesharing representative. Thus the public software can be used on private files.

The reverse is also true and can be of interest to many users. That is, one can develop new software or modify the existing software for searching or manipulating the public data base. In fact, it is the hope of the designers of the system that there will be an evolution of software developments that will be made available to all users of the system around the world for their testing, evaluation and possible use. All of the software currently on the system is in the public domain and available on a non-exclusive basis to any and all interested parties, so long as they do

not profit from the software (such as reselling the software provided free).

APPENDIX A

Account Information

To obtain an account on the GE MARK III Timesharing network please contact the office listed in Appendix C nearest to you. If there are any problems please contact:

MSSS Marketing Representative
GE, Suite 1036
777 14th Street, N. W.
Washington, D. C. 20005 USA
(202) 628-4000

To obtain an account on the NIH DCRT/CCB PDP-10, please contact:

Mr. Henry J. Juenemann
Assistant Director
Bldg. 12A, Rm. 3029
DCRT, NIH
Bethesda, Maryland 20014
(301) 496-2282

APPENDIX B

USER ASSISTANCE

The best way to contact someone regarding the system is by using the CRAB option. This does away with the need for long distance phone calls, secretaries and postal systems. However, human nature being what it is, here are the people, their addresses and telephone numbers, to contact:

1. MSDC - regarding royalties, data base and and microfiche for the GE system:

MSDC MSSS Staff
Bldg. A8.1A
MSDC, AWRE
Aldermaston, Reading, RG7 4PR
Britain (UK)
073-56-4111, ext. 5852

2. GE - a) regarding GE network problems unsolvable or unanswerable locally:

MSSS Marketing Representative
GE, Suite 1036
777 14th Street, N.W.
Washington, D. C. 20005 USA
(202) 628-4000

b) regarding program problems and proprietary files.

Ms. Rachelle Heller
University College
Computer Science Department
University of Maryland
College Park, Maryland 20742 USA

3. NIH - a) regarding PDP-10 program problems

Ms. Alice Bridy
Bldg. 12A, Rm. 2001
DCRT, NIH
Bethesda, Maryland 20014 USA
(301) 496-5693

b) regarding technical mass spec questions

Drs. Henry M. Fales or Bill Milne
Bldg. 10, Rm. 7N-306
NHLI, NIH
Bethesda, Maryland 20014 USA
(301) 496-2135 or (301) 496-3341

4. EPA - regarding EPA user questions:

Dr. John McGuire
EPA, Southeast Envirnomental Research Laboratory
College Station Road
Athens, Georgia 30601 USA
(404) 546-3185

Dr. Stephen R. Heller
EPA, HIDSD, PM-218
401 M St., S. W.
Washington, D. C. 20460 USA
(202) 755-0811

APPENDIX C

GE MARK III Timesharing System Network Telephone Information

UNITED STATES

	COMPUTER ACCESS	CUSTOMER SERVICE
ALABAMA		
ANNISTON	(205) 237-1678	(615) 259-4571
BIRMINGHAM	(205) 328-4020	(404) 256-1794*
DOTHAN	(205) 794-8679	1-800-845-0108
FLORENCE	(205) 766-7963	(615) 259-4571*
HUNTSVILLE	(205) 539-7733	(615) 259-4571*
MOBILE	(205) 433-7463	(504) 837-0722
MOULTON	(205) 974-1128	(615) 259-4571*
MUSCLE SHOALS	(205) 381-0172	(615) 259-4571*
OPELIKA	(205) 749-2096	(615) 259-4571*
TUSCALOOSA	(205) 759-4492	(615) 259-4571*
ALASKA		
ANCHORAGE	(907) 279-9561	(206) 763-0850
ARIZONA		
PHOENIX	(602) 263-1111	(602) 264-7884*
TUCSON	(602) 884-7300	(602) 264-7884*
ARKANSAS		
LITTLE ROCK	(501) 376-4636	(615) 259-4571*
CALIFORNIA		
AGOURA	(213) 889-2280	(213) 783-8970*
BAKERSFIELD	(805) 327-1461	(805) 687-5368
BERKELEY	(415) 486-6700	(415) 989-1100*
BORON	(714) 762-6131	(213) 783-8970*
COMPTON	(213) 537-7650	(213) 426-9345
CONCORD	(415) 825-9111	(415) 989-1100*
ELMONTE	(213) 579-6440	(213) 426-9345*
LOMPOC	(805) 736-8589	(805) 687-5368
LOS ANGELES	(213) 778-7222	(213) 385-9411*
MODESTO	(209) 529-8055	(415) 969-3772*
OAKLAND	(415) 465-6700	(415) 989-1100*
ONTARIO	(714) 983-9841	(213) 426-9345*
OXNARD	(805) 487-0643	(213) 783-8970*
REDWOOD CITY	(415) 364-0900	(415) 969-3772*
RIALTO	(714) 875-8751	(213) 426-9345*
RICHMOND	(415) 849-0161	(415) 989-1100*
SACRAMENTO	(916) 444-3003	(916) 442-1696
SAN DIEGO	(714) 291-9880	(714) 232-7167
SAN FRANCISCO	(415) 465-6700	(415) 989-1100*
S. SAN FRANCISCO	(415) 811-9811	(415) 989-1100*
W. SAN FRANCISCO	(415) 433-4211	(415) 989-1100*
SAN RAFAEL	(415) 454-5300	(415) 989-1100*
SANTA ANA	(714) 836-4901	(213) 426-9345*
SANTA BARBARA	(805) 963-6811	(805) 687-5368
SANTA MONICA	(213) 398-2741	(213) 783-8970*
SUNNYVALE	(408) 738-3535	(415) 969-3772*
UNION CITY	(415) 489-9400	(415) 969-3772*
VICTORVILLE	(714) 245-1865	(213) 426-9345*
COLORADO		
COLORADO SPRINGS	(303) 471-3530	(303) 388-5751*
DENVER	(303) 534-1122	(303) 388-5751*
DILLON	(303) 468-6110	(303) 388-5751*
LOVELAND	(303) 669-1020	(303) 388-5751*
FORT COLLINS	(303) 493-4474	(303) 388-5751*
CONNECTICUT		
BLOOMFIELD	(203) 243-8901	(203) 289-7941*
BRIDGEPORT	(203) 377-6707	(203) 289-7941*
GROTON	(203) 445-7486	(203) 289-7941*
HARTFORD	(203) 278-0650	(203) 289-7941*
NEW HAVEN	(203) 772-0630	(203) 289-7941*
STAMFORD	(203) 359-3400	(203) 289-7941*
SAYBROOK	(203) 388-5833	(203) 289-7941*
WESTPORT	(203) 838-8461	(203) 289-7941*
DELAWARE		
WILMINGTON	(302) 652-3074	(800) 638-0822
DISTRICT OF COLUMBIA		
WASHINGTON	(301) 652-4445	(301) 657-2120*
WASHINGTON	(301) 656-1920	(301) 657-2120*
WASHINGTON	(301) 656-2720	(301) 657-2120*
FLORIDA		
F. WALTON BEACH	(904) 244-2310	(504) 837-0722
FORT LAUDERDALE	(305) 524-5593	(305) 989-7557
GAINSVILLE	(904) 373-3367	(813) 877-8294
JACKSONVILLE	(904) 358-3915	(305) 894-6101
LAKELAND	(813) 688-5261	(813) 877-8294
MELBOURNE	(305) 724-4660	(305) 894-6101
MIAMI	(305) 358-2390	(305) 621-1196*
OCALA	(904) 732-3700	(305) 894-6101
ORLANDO	(305) 841-4310	(305) 894-6101
PENSACOLA	(904) 432-0916	(504) 837-0722
ST. PETERSBURG	(813) 822-1212	(813) 877-8294
TAMPA	(813) 236-5583	(813) 877-8294
VERO BEACH	(305) 562-1674	(305) 989-7557
W. PALM BEACH	(305) 833-3731	(305) 989-7557
GEORGIA		
ALBANY	(912) 436-6153	(404) 256-1794*
ATHENS	(404) 549-8513	(404) 256-1794*
ATLANTA	(404) 875-7351	(404) 256-1794*
AUGUSTA	(404) 722-2262	1-800-845-0108
CARROLTON	(404) 834-6841	(404) 256-1794*
DALTON	(404) 226-7744	(404) 256-1794*
MACON	(912) 745-7437	(404) 256-1794*
MOULTRIE	(912) 985-8581	(404) 256-1794*
NEWNAN	(404) 253-8482	(404) 256-1794*
SAVANNAH	(912) 233-2117	1-800-845-0108
ROME	(404) 235-8031	(404) 256-1794*
IDAHO		
BOISE	(208) 344-5876	(503) 288-6915
IDAHO FALLS	(208) 523-8220	(303) 388-5751
KELLOGG	(208) 784-1111	(208) 763-0850
NAMPA	(208) 467-3326	(503) 288-6915
ILLINOIS		
BLOOMINGTON	(309) 829-5361	(314) 436-4343**
CHICAGO	(312) 346-8484	(312) 663-3900*
DECATUR	(217) 429-0192	(314) 436-4343**
MORRISON	(815) 772-7251	(612) 544-6838*
PEORIA	(309) 673-6071	(314) 436-4343**
QUINCY	(217) 224-2910	(314) 436-4343**
ROCKFORD	(815) 962-5062	(312) 663-3900*
INDIANA		
BLOOMINGTON	(812) 336-0281	(317) 545-7591*
COLUMBUS	(812) 372-3711	(317) 545-7591*
ELKHART	(219) 294-5438	(317) 545-7591*
EVANSVILLE	(812) 425-4331	(800) 638-0822
FORT WAYNE	(219) 422-8487	(317) 545-7591*
INDIANAPOLIS	(317) 545-4261	(317) 545-7591*
LAFAYETTE	(317) 423-1691	(317) 545-7591*
MUNCIE	(317) 289-6386	(317) 545-7591*
RICHMOND	(317) 966-7675	(317) 966-7675
SOUTH BEND	(219) 289-7011	(317) 545-7591*
TERRE HAUTE	(812) 235-8031	(317) 545-7591*
IOWA		
BURLINGTON	(319) 754-5771	(612) 544-6838
DAVENPORT	(319) 326-0136	(612) 544-6838
DES MOINES	(515) 280-8861	(612) 544-6838
KANSAS		
WICHITA	(316) 262-0415	(405) 947-2376
COFFEYVILLE	(316) 251-7600	(918) 743-9761
McPHERSON	(316) 241-0348	(405) 947-2376
KENTUCKY		
BOWLING GREEN	(502) 842-8118	(800) 638-0822
LEXINGTON	(606) 233-0521	(800) 638-0822
LOUISVILLE	(502) 589-3820	(800) 638-0822
OWENSBORO	(502) 685-3125	(800) 638-0822
LOUISIANA		
BATON ROUGE	(504) 348-2251	(504) 837-0724
LAFAYETTE	(318) 233-4610	(504) 837-0724
LAKE CHARLES	(318) 436-3681	(713) 771-7292
NEW ORLEANS	(504) 837-1910	(504) 837-0724
SHREVEPORT	(318) 425-2463	(318) 425-2476
MAINE		
AUGUSTA	(207) 622-9341	(617) 926-2911*
BANGOR	(207) 947-0591	(617) 926-2911*
KITTERY	(207) 439-4100	(617) 926-2911*
MARYLAND		
BALTIMORE	(301) 685-1570	(301) 323-8700
BETHESDA	(301) 656-2720	(301) 657-2120*
BETHESDA	(301) 652-4445	(301) 657-2120*
BETHESDA	(301) 656-1920	(301) 657-2120*
CUMBERLAND	(301) 724-8490	(301) 657-2120*
SALISBURY	(301) 749-8388	(301) 657-2120
MASSACHUSETTS		
ATTLEBORO	(617) 226-1150	(617) 926-2911*
BOSTON	(617) 950-6900	(617) 926-2911*
FALL RIVER	(617) 679-8121	(617) 926-2911*
FALMOUTH	(617) 548-7150	(617) 926-2911*
FITCHBURG	(617) 345-7585	(617) 926-2911*
HYANNIS	(617) 775-0752	(617) 926-2911*
LYNN	(617) 594-6411	(617) 926-2911*

*24 hour customer service is available. In case of trouble on the assigned line, during after hours and weekends, dial inwats number 800-321-2330 for customer service.

	COMPUTER ACCESS	CUSTOMER SERVICE
MASSACHUSETTS		
NEEDHAM	(617) 449-1021	(617) 926-2911*
NORTH ADAMS	(413) 664-6787	(413) 494-4308
NORTHAMPTON	(413) 586-2320	(413) 494-4308
PITTSFIELD	(413) 494-5161	(413) 494-4308
SOUTHBRIDGE	(617) 765-5493	(617) 926-2911*
SPRINGFIELD	(413) 781-5854	(203) 289-7941
WORCESTER	(617) 757-3862	(617) 926-2911*
MICHIGAN		
ANN ARBOR	(313) 769-6330	(313) 968-8100*
BATTLE CREEK	(616) 968-8121	(313) 968-8100*
BENTON HARBOR	(616) 926-7275	(313) 968-8100*
DETROIT	(313) 568-2810	(313) 968-8100*
FLINT	(313) 767-7865	(313) 968-8100*
GRAND RAPIDS	(616) 459-6183	(313) 968-8100*
KALAMAZOO	(616) 382-4241	(313) 968-8100*
LANSING	(517) 372-3130	(313) 968-8100*
MUSKEGON	(616) 722-7815	(313) 968-8100*
ROYAL OAK	(313) 968-1450	(313) 968-8100*
SAGINAW	(517) 799-8480	(313) 968-8100
MINNESOTA		
MINNEAPOLIS	(612) 377-9960	(612) 544-6838**
MISSISSIPPI		
GULFPORT	(601) 863-2246	(504) 837-0722
JACKSON	(601) 948-3193	(504) 837-0722
VICKSBURG	(601) 638-5640	(504) 837-0722
MISSOURI		
BONNE TERRE	(314) 358-3368	(314) 436-4343**
KANSAS CITY	(816) 753-5133	(314) 436-4343**
ST. LOUIS	(314) 436-6720	(314) 436-4343**
MONTANA		
BOZEMAN	(406) 587-4567	(303) 388-5751
NEBRASKA		
OMAHA	(402) 344-0700	(612) 544-6838*
NEVADA		
LAS VEGAS	(702) 382-6810	(602) 264-7804
NEW HAMPSHIRE		
NASHUA	(603) 883-4133	(617) 926-2911*
ROCHESTER	(603) 332-8110	(617) 926-2911
NEW JERSEY		
EATONTOWN	(201) 542-4080	(201) 675-2155*
HURFFVILLE	(609) 589-5222	(201) 675-2155*
MERCHANTVILLE	(609) 665-5260	(800) 638-0822*
MILLVILLE	(609) 825-7200	(201) 675-2155*
MORRISTOWN	(201) 267-4090	(201) 675-2155*
NEW BRUNSWICK	(201) 249-1853	(201) 675-2155*
ORANGE	(201) 672-5431	(201) 675-2156*
PRINCETON	(609) 924-9240	(201) 675-2156*
RAHWAY	(201) 382-7011	(201) 675-2155*
RAMSEY	(201) 825-1030	(201) 675-2156*
RUTHERFORD	(201) 935-7100	(201) 675-2156*
SUMMIT	(201) 464-6111	(201) 675-2155*
TEANECK	(201) 837-7031	(201) 675-2155*
TOMS RIVER	(201) 349-7075	(800) 638-0822
NEW MEXICO		
ALBUQUERQUE	(505) 843-6600	(505) 298-7591
SANTA FE	(505) 983-6305	(505) 298-7591
NEW YORK		
AMSTERDAM	(518) 842-4720	(518) 372-5471*
AUBURN	(315) 253-4483	(315) 456-1995
BINGHAMTON	(607) 723-7901	(607) 772-0546
BUFFALO	(716) 881-0550	(800) 638-0822
CORNING	(607) 962-5041	(315) 456-1995*
CORTLAND	(607) 753-9374	(315) 456-1995*
COXSACKIE	(518) 731-6141	(518) 372-5471*
DEER PARK	(516) 667-0100	(212) 832-5856
ELMIRA	(607) 734-4221	(315) 456-1995*
FULTON	(315) 592-9541	(315) 456-1995*
GENEVA	(315) 789-9800	(315) 456-1995*
GLEN FALLS	(518) 793-5603	(518) 372-5471*
HERKIMER	(315) 866-3910	(315) 456-1995*
JAMESTOWN	(716) 488-0773	(716) 837-7752
MEXICO	(315) 963-7249	(315) 456-1995*
MINEOLA	(516) 248-1380	(212) 832-5856
NEW YORK CITY	(212) 551-9711	(212) 832-5856
NEW YORK CITY	(212) 564-9120	(212) 832-5856
NEW YORK CITY	(212) 765-8710	(212) 832-5856
NIAGARA FALLS	(716) 285-3638	(716) 837-7752
NEW YORK		
NORWICH	(607) 334-5620	(315) 456-1995*
NYACK	(914) 358-9177	(212) 832-5856
OSWEGO	(315) 342-4127	(315) 456-1995*
PORT JEFFERSON	(516) 928-9033	(212) 832-5856
PORT JEFFERSON	(516) 928-9033	(201) 675-2155
POUGHKEEPSIE	(914) 454-5620	(518) 372-5471*
ROCHESTER	(716) 546-7600	(800) 638-0822
SCHENECTADY	(518) 370-1000	(518) 372-5471*
SYRACUSE	(315) 463-6291	(315) 456-1995*
UTICA	(315) 797-6550	(315) 456-1995*
WATERTOWN	(315) 788-7740	(315) 456-1995*
WHITE PLAINS	(914) 428-6150	(212) 832-5856
WOODSTOCK	(914) 679-2445	(518) 372-5471*
NORTH CAROLINA		
ASHEVILLE	(704) 253-2761	1-800-845-0106
BREVARD	(704) 883-8275	1-800-845-0106
BURLINGTON	(919) 227-9031	1-800-845-0106
CHARLOTTE	(704) 525-8580	1-800-845-0106
DURHAM	(919) 682-8121	1-800-845-0106
ELKIN	(919) 835-7198	1-800-845-0106
GASTONIA	(704) 867-0261	1-800-845-0106
GREENSBORO	(919) 697-8800	1-800-845-0106
HENDERSONVILLE	(704) 692-0517	1-800-845-0106
HIGH POINT	(919) 886-5038	1-800-845-0106
KANNAPOLIS	(704) 932-6151	1-800-845-0106
MOCKSVILLE	(704) 634-5971	1-800-845-0106
MT. AIRY	(919) 789-5146	1-800-845-0106
LENOIR	(704) 758-9151	1-800-845-0106
NEWTON	(704) 464-7840	1-800-845-0106
PLYMOUTH	(919) 793-5141	1-800-845-0106
RALEIGH	(919) 833-7351	1-800-845-0106
REIDSVILLE	(919) 349-2301	1-800-845-0106
RUTHERFORDTON	(704) 286-9168	1-800-845-0106
SALISBURY	(704) 633-7250	1-800-845-0106
WILMINGTON	(919) 763-3605	1-800-845-0106
WINSTON-SALEM	(919) 722-6391	1-800-845-0106
NORTH DAKOTA		
BISMARCK	(701) 255-0972	(612) 544-6838
OHIO		
AKRON	(216) 379-9500	(800) 638-0822
CANTON	(216) 452-9876	(800) 638-0822
CINCINNATI	(513) 721-5599	(800) 638-0822
CLEVELAND	(216) 433-7500	(800) 638-0822
CLEVELAND	(216) 267-8150	(800) 638-0822
COLUMBUS	(614) 228-7741	(800) 638-0822
COSHOCTON	(614) 622-0011	(800) 638-0822
DAYTON	(513) 223-7174	(800) 638-0822
DEFIANCE	(419) 782-9700	(800) 638-0822
LIMA	(419) 228-7212	(800) 638-0822
MANSFIELD	(419) 526-1014	(800) 638-0822
MARION	(614) 382-9947	(800) 638-0822
MIDDLETOWN	(513) 424-5358	(800) 638-0822
SPRINGFIELD	(513) 323-4605	(800) 638-0822
TOLEDO	(419) 242-7351	(800) 638-0822
TROY	(513) 339-3412	(800) 638-0822
WARREN	(216) 399-6455	(800) 638-0822
YOUNGSTOWN	(216) 744-5081	(800) 638-0822
OKLAHOMA		
BARTLESVILLE	(918) 336-8500	(918) 743-9761*
DUNCAN	(405) 252-0930	(405) 947-2376
OKLAHOMA CITY	(405) 272-9581	(405) 947-2376
PONCA CITY	(405) 762-7511	(405) 947-2376
TULSA	(918) 581-0211	(918) 743-9761*
OREGON		
ALBANY	(503) 926-2252	(503) 288-6915
PORTLAND	(503) 288-7551	(503) 288-6915
PENNSYLVANIA		
ALLENTOWN	(215) 439-0423	(800) 638-0822
BUTLER	(412) 283-1111	(800) 638-0822
CHESTER	(215) 874-5387	(800) 638-0822
COATESVILLE	(215) 384-6050	(800) 638-0822
CRESSON	(814) 886-4121	(800) 638-0822
ERIE	(814) 453-3641	(800) 638-0822
ERIE	(814) 459-1755	(800) 638-0822
HARRISBURG	(717) 238-9311	(800) 638-0822
HAZELTON	(717) 455-9533	(800) 638-0822

*24 hour customer service is available. In case of trouble on the assigned line, during after hours and weekends, dial inwats number 800-321-2330 for customer service, except for state of Ohio dial inwats 800-362-2929.

	COMPUTER ACCESS	CUSTOMER SERVICE
PENNSYLVANIA		
LANCASTER	(717) 397-2466	(800) 638-0822
LANGHORNE	(215) 752-0328	(800) 638-0822
PHILADELPHIA	(215) 629-9700	(800) 638-0822
PITTSBURGH	(412) 323-0900	(800) 638-0822
PORTAGE	(814) 736-8934	(800) 638-0822
READING	(215) 372-4751	(800) 638-0822
WILLIAMSPORT	(717) 323-9645	(800) 638-0822
YORK	(717) 845-7641	(800) 638-0822
RHODE ISLAND		
PROVIDENCE	(401) 351-6024	(617) 926-2911*
SOUTH CAROLINA		
AIKEN	(803) 648-2676	(803) 233-5335
ANDERSON	(803) 225-1676	(803) 233-5335
CHARLESTON	(803) 722-3388	(803) 233-5335
CLEMSON	(803) 654-2433	(803) 233-5335
COLUMBIA	(803) 256-4315	(803) 233-5335
GREENVILLE	(803) 242-3485	(803) 233-5335
GREENWOOD	(803) 229-0464	(803) 233-5335
LANCASTER	(803) 285-6911	(803) 233-5335
LAURENS	(803) 682-3251	(803) 233-5335
ROCK HILL	(803) 327-1126	(803) 233-5335
SPARTANBURG	(803) 585-6771	(803) 233-5335
TENNESSEE		
CHATTANOOGA	(615) 267-4581	(404) 256-1794*
KINGSPORT	(615) 246-7444	(404) 256-1794*
KNOXVILLE	(615) 546-6513	(404) 256-1794*
MEMPHIS	(901) 527-9316	(615) 259-4571
MURFREESBORO	(615) 893-3734	(615) 259-4571
NASHVILLE	(615) 244-6262	(615) 259-4571
TEXAS		
AUSTIN	(512) 476-6046	(713) 771-7292
BROWNSVILLE	(512) 542-9175	(713) 771-7292
CORPUS CHRISTI	(512) 888-4421	(713) 771-7292
DALLAS	(214) 522-5210	(214) 631-0910*
EL PASO	(915) 532-1831	(505) 298-7591
FORT WORTH	(214) 263-5271	(214) 631-0910*
GRAND PRAIRIE	(214) 263-5271	(214) 631-0910*
HOUSTON	(713) 223-5474	(713) 771-7292
LUFKIN	(713) 634-2502	(318) 425-2478
MARSHALL	(214) 938-8361	(318) 425-2478
MIDLAND	(915) 563-0355	(713) 771-7292
ORANGE	(713) 886-6601	(713) 771-7292
PORT LAVACA	(512) 552-6706	(713) 771-7292
PORT NECHES	(713) 727-3591	(713) 771-7292
SAN ANGELO	(915) 655-6915	(713) 771-7292
SAN ANTONIO	(512) 224-4425	(713) 771-7292
SEMINOLE	(915) 758-5873	(713) 771-7292
SHERMAN	(214) 892-1991	(214) 631-0910
SNYDER	(915) 573-6531	(713) 771-7292
TERMINAL	(915) 563-0355	(713) 771-7292
TYLER	(214) 595-1071	(214) 631-0910
UTAH		
OGDEN	(801) 621-4910	(303) 388-5751
SALT LAKE CITY	(801) 521-7220	(303) 388-5751
VERMONT		
BRATTLEBORO	(802) 257-0571	(518) 372-5471*
BURLINGTON	(822) 658-0110	(518) 372-5471*
MONTPELIER	(802) 223-2316	(518) 372-5471*
SPRINGFIELD	(802) 885-5721	(518) 372-5471*
VIRGINIA		
CHESTER	(804) 748-6406	(800) 638-0822
HARRISONBURG	(703) 434-1786	(800) 638-0822
HERNDON	(703) 437-0500	(800) 638-0822
LYNCHBURG	(804) 845-3441	(800) 638-0822
MARTINSVILLE	(703) 632-9705	(800) 638-0822
NEWPORT NEWS	(804) 244-0141	(800) 638-0822
NORFOLK	(804) 623-9171	(800) 638-0822
RESTON	(703) 437-0500	(800) 638-0822
RICHMOND	(804) 644-0344	(800) 638-0822
ROANOKE	(703) 345-0435	(800) 638-0822
WAYNESBORO	(703) 942-0181	(800) 638-0822
WASHINGTON		
EVERETT	(206) 355-2511	(206) 575-2990*
OLYMPIA	(206) 943-5200	(206) 575-2990*

	COMPUTER ACCESS	CUSTOMER SERVICE
WASHINGTON		
SEATTLE	(206) 575-2950	(206) 575-2990*
SPOKANE	(509) 328-9400	(206) 575-2990*
TACOMA	(206) 927-0104	(206) 575-2990*
WEST VIRGINIA		
BLUEFIELD	(304) 325-6451	(800) 638-0822
BRANDYWINE	(304) 249-5341	(800) 638-0822
CHARLESTON	(304) 344-3546	(800) 638-0822
WHEELING	(304) 232-6600	(800) 638-0822
WISCONSIN		
APPLETON	(414) 739-0244	(414) 271-7900
MADISON	(608) 257-0245	(414) 271-7900
MILWAUKEE	(414) 271-7980	(414) 271-7900
RACINE	(414) 637-9721	(414) 271-7900
WYOMING		
CASPER	(307) 265-7287	(303) 388-5751

*24 hour customer service is available. In case of trouble on the assigned line, during after hours and weekends, dial inwats number 800-321-2330 for customer service.

INTERNATIONAL

Outside the United States, MARKIII service is available through our Authorized Distributors.

	DISTRIBUTOR CONTACT LIST	CUSTOMER SERVICE
AUSTRALIA		
MANAGER, TIME-SHARING HONEYWELL INFORMATION SYSTEMS 863 BOURKE STREET WATERLOO (SYDNEY), NSW 2017 PHONE: 69.0355		
MANAGER, TIME-SHARING HONEYWELL INFORMATION SYSTEMS 350 ST. KILDA ROAD MELBOURNE, VICTORIA 3004 699-3288		
* SYDNEY		69-0355
* MELBOURNE		699-3288
AUSTRIA		
SALES MANAGER HONEYWELL BULL OBERE DONAUSTRASSE 49.51 1020 VIENNA PHONE: 222-33-41-51		
* VIENNA		222-33-41-51
BELGIUM		
SALES MANAGER GENERAL TIME-SHARE AVENUE DES ARTS 56 1040 BRUSSELS PHONE (02) 11.07.40		
* BRUSSELS		(02) 11.07.40

Computer access numbers for the cities indicated are available on request by calling the listed customer service number.

*Indicates availability of 30 CPS service

	DISTRIBUTOR CONTACT LIST	CUSTOMER SERVICE

CANADA

INFORMATION SERVICES
CANADIAN GENERAL ELECTRIC CO. LTD.
1420 DUPONT STREET
TORONTO M6H2B2 ONTARIO
PHONE (416) 534-6511

ALBERTA

*	CALGARY	(403) 266-7311
*	EDMONTON	(403) 429-6757

BRITISH COLUMBIA

*	VANCOUVER	(604) 681-8136

ONTARIO

*	OTTAWA	(613) 722-6511
*	TORONTO	(416) 534-6511

QUEBEC

*	MONTREAL	(514) 866-1884

DENMARK

T/S MANAGER
ØK DATA
VESTERBROGADE 1
DK – 1620 COPENHAGEN V
PHONE 01 1222.00

*	COPENHAGEN	01 12 32 00

FRANCE

SALES MANAGER
COMPAGNIE HONEYWELL BULL
179-181 AV. CHARLES DE GAULLE
92 NEUILLY
PHONE 747-7042

	BORDEAUX	(15) 56 44 82 73
	LE HAVRE	(16) 35 98 18 98
*	LILLE	747-7042
*	LYON	(15) 78 28 56 82
	MARSEILLE	(15) 91 77 88 83
	NANCY	(15) 28 27 01 96
	NICE	(15) 91 77 88 83
*	PARIS	747-7042
	ROUEN	(16) 35 98 18 98
	STRASBOURG	(15) 28 27 01 96
	TOULOUSE	(15) 56 44 82 73

ITALY

TIME-SHARING MANAGER
HONEYWELL INFORMATION SYSTEMS ITALIA
VIA M. GIOIA, 70
20125 MILAN
PHONE 688-6541

*	BOLOGNA	277-881
*	FLORENCE	688-6541
*	MILAN	688-6541
*	NAPLES	688-6541
	PADUA	662-911
*	ROME	479-051
*	TURIN	540-058
	GENOA	688-6541

JAPAN

SALES MANAGER, TIME SHARING
DENTSU ADVERTISING, LTD.
11, 1-CHOME, TSUKIJI, TOKYO. 104
PHONE (03) 544-7257

*	NAGOYA	(03) 544-7257
*	OSAKA	(03) 544-7257
*	TOKYO	(03) 544-7257

NETHERLANDS

SALES MANAGER
HONEYWELL BULL (NEDERLAND) N.V.
VLIEGTUIGSTRAAT 36
AMSTERDAM
PHONE 020-158955

*	THE HAGUE	020-158955

PUERTO RICO

COMPUTER SYSTEMS OF PUERTO RICO, INC.
LA CERAMICA INDUSTRIAL PARK
BLDG. 6
CALLE GILDITA
CAROLINA
PHONE 768-6108

*	SAN JUAN	(809) 768-6108

SWEDEN

SALES MANAGER
HONEYWELL BULL AB
BOX 23137 S-104 35
STOCKHOLM 23
PHONE 24-88-20

*	STOCKHOLM	24 88 20
*	GOTEBORG	12 42 35
	MALMO	7 36 25

SWITZERLAND

TIME-SHARING MANAGER
HONEYWELL BULL (SCHWEIZ) AG
HARDTURMSTRASSE 253
CH8006 ZURICH

*	ZURICH	01-44. 49. 40

UNITED KINGDOM

SALES MANAGER, TIME SHARING
HONEYWELL INFORMATION SYSTEMS LTD.
114-118 SOUTHAMPTON ROW
LONDON, W.C. 1
PHONE (01)-242-5725

ENGLAND

*	BIRMINGHAM	021-373-8144
*	LEEDS	061-486-6116
*	LIVERPOOL	061-486-6116
*	LONDON	(01) 242-5725
*	MANCHESTER	061-486-6116
*	NEWCASTLE	0386-63021
*	SOUTHAMPTON	(01) 242-5725

SCOTLAND

*	EDINBURGH	041-882-8244
*	GLASGOW	041-882-8244

WALES

*	CARDIFF	0272-292831/5

WEST GERMANY

SALES MANAGER
HONEYWELL BULL GmbH
HOHENSTAUFENRING 62
5000 KOELN
PHONE 0221-20371

COLOGNE	02 21-20371
FRANKFURT	06196-4711
HAMBURG	040-2201378
STUTTGART	0711-223463

*Indicates availability of 30 CPS service

Computer access numbers for the cities indicated are available on request by calling the listed customer service number.

APPENDIX D

MSDC COMPOUND CLASSIFICATION CODES

Code #	Description		
1000	Hydrocarbon (and skeleton)	Alkane	
1010	"	Alkene	
1020	"	Alkyne	
1030	"	Alicyclic	Monocyclic (including cyclenes)
1040	"	"	Fused and Spirocyclic
1050	"	Aromatic	Monocyclic
1060	"	"	Fused
1070	"	Alicyclic/Aromatic fused	
1080	"	Other	
1090	Heterocyclic Nitrogen		
1100	" Oxygen		
1110	" Sulphur		
1120	" Other		
1130	Oxygen function	Hydroxyl	
1140	" "	Ether, Orthoester, Peroxide	Not heterocyclic oxygen, acetal or ketal
1150	" "	Acetal	
1160	" "	Ketal	
1170	" "	Aldehyde	
1180	" "	Ketone, Ketene Quinone	
1190	" "	Carboxylic acid	
1200	" "	Acid anhydride	
1210	" "	Ester, not methyl ester	
1220	" "	Methyl ester	
1230	" "	Acid salt	
1240	" "	Lactone	
1250	" "	Acid halide	
1260	" "	Amide, Imide, Urea	
1270	" "	Lactam	
1280	" "	Other	
1290	Nitrogen function	Amine, Imine	
1300	" "	Nitrile, isonitrile, isocyanate, Isothiocyanate	
1310	" "	Nitro, Nitroso, Nitrate, Nitrite, oxime, N-oxide	
1320	" "	Hydrazine, Azo, Diazo, Azide	
1330	" "	Other	
1340	Sulphur function	Thiol, sulphide	
1350	" "	Thione	
1360	" "	Sulphone, sulphoxide, sulphonic acid and ester	

1370	"	"	Thiocarboxylic acid and ester
1380	"	"	Other
1390	Halogen		Fluorine
1400	"		Chlorine
1410	"		Bromine
1420	"		Iodine
1430	Other non-metal		Phosphorus-trivalent
1440	"		Phosphorus pentavalent
1450	"		Trimethylsilyl
1460	"		Silicon, not TMS
1470	"		Boronate
1480	"		Boron, not boronate
1490	"		Other
1500	Metal"		Group IA (Li, Na, K, Rb, Cs, Fr)
1510	"		Group IB (Cu, Ag, Au)
1520	"		Group IIA (Be, Mg, Ca, Sr, Ba, Ra)
1530	"		Group IIB (Zn, Cd, Hg)
1540	"		Group IIIA Not lanthanide, actinide (Sc, Y)
1550	"		Lanthanide
1560	"		Actinide
1570	"		Group IIIB (Al, Ga, In, Tl)
1580	"		Group IVA (Ti, Zr, Hf)
1590	"		Group IVB (Ge, Sn, Pb)
1600	"		Group VA (V, Nb, Ta)
1610	"		Group VIA (CR, Mo, W)
1620	"		Group VIIA (Mn, Tc, Re)
1630	"		Group VIII (Fe, Co, Ni, Ru, Rh, Pd, Os, Ir, Pt)
1640	"		Organo-metallic carbonyl
1650	Natural Product		Alkaloid
1660	"	"	Amino acid, Peptide, Protein
1670	"	"	Carbohydrates
1680	"	"	Flavanoid, Anthocyanin, Chroman
1690	"	"	Mycoside
1700	"	"	Nucleic acid, nucleotide, Nucleoside
1710	"	"	Steroid
1720	"	"	Terpenoid Mono-
1730	"	"	" Sesqui
1740	"	"	" Di-
1750	"	"	" Tri
1760	"	"	" Higher
1770	"	"	" Isoprenoid
1780	"	"	Carotenoid
1790	"	"	Porphyrin
1800	"	"	Chlorin
1810	"	"	Phospho-lipid
1820	"	"	Other
1830	Special Class		Polymer
1840	"	"	D-labelled
1850	"	"	Otherwise labelled

APPENDIX E

NIH MSSS MASS SPECTRAL DATA BASE FILE FORMAT

For those users wishing to contribute spectra to the system, the following format has been adopted for the master file. For those users on the GE network who plan to put up their own propietary data base, this information will be helpful in preparing their files.

The master mass spec file starts out as two basic files.

1. Data File
2. Info File

I. Data

RECFM=FB, LRECL=21, BLKSIZE=2100

1 record per peak 1X,I5,1X,I4,1X,I4,1X,I4

I5 Spectrum identification number

I4 Total number of peaks

I4 m/e (integral)

I4 Relative Intensity (normalized to 10000, but biggest peaks 9999)

All peaks with zero intensity or non-integral m/e or metastable are omitted.

II. Information

RECFM=FB, LRECL=80, BLKSIZE=800

8 records per spectrum, each record begining 1X,I5,1X,I1,1X

I5 Spectrum identification number

I1 Record number (1 to 8)

Items not available are blank for A mode, zero (right-adjusted) for I mode

Record 1: I4,1X,26A1,1X,2A4,A2,2A4,A2,3I3,A4,2I2,2X

1I4 Molecular Weight (integral)

26A1 Formula

2A4,A2 Instrument

2A4,A2 Inlet type

I3 Inlet temperature

I3 Source temperature

I3 Electron voltage

A4 Ion accelerating voltage

2I2 Pressure (eg 1.7 x 10-5 as 17-5)

Record 2: A3,1I5,62A1

A3 Spectrum collection letters (eg MSC, API etc)

I5 Collection number

62A1 Contributor

Records 3,4,5: 70A1,1X

Compound name (210 characters allowed)

Record 6: 1X,1I9,1X,60A1

1I9 CAS Registry Number (REGN)

60A1 WLN

Record 7: 71A1

WLN (continued)

Record 8: 12I4,1X,22A1

12I4 MSDC Compound Classifications

22A1 WLN (Continued - 153 characters allowed)

Both these files must be worked over to produce files that the file generation program on the PDP-10/GE-635 can use.

MASS DATA COLLECTION SHEET

Please forward completed form to:

Dr. Stephen R. Heller
EPA, PM-218
401 M St., S.W.
Washington, D.C. 20460

Please fill out this form as completely as possible. The data will be converted into computer readable form and a listing returned to you for approval. All data submitted will be considered in the public domain. It may not be reproduced in any form for profit.

1 INFO

Name:

Address:

Phone:

Your ID code for sample:

Compound Name:

CAS REGN:

WLN:

Molecular Formula:

Molecular Weight:

MSDC Codes:

MS Instrument:

Inlet System:

GC column type and gas:

Inlet Temp (^{O}C):

Source Temp (^{O}C):

Ionizing Voltage (EV):

ion Accel. Voltage (KV):

Pressure (Torr):

STRUCTURE

2 DATA

Intensities (Int.) range from 0.000% to 100.00%, but the largest peak (m/e) is 9999. All intensities are written without the decimal point. Eg. 15.43% is written as 1543 1% is written as 100 and 0.1% is written as 10.

m/e	Int.	m/e	Int.	m/e	Int.	m/e	Int.	m/e	Int.	m/e	Int.
12		47		82		117		152		187	
13		48		83		118		153		188	
14		49		84		119		154		189	
15		50		85		120		155		190	
16		51		86		121		156		191	
17		52		87		122		157		192	
18		53		88		123		158		193	
19		54		89		124		159		194	
20		55		90		125		160		195	
21		56		91		126		161		196	
22		57		92		127		162		197	
23		58		93		128		163		198	
24		59		94		129		164		199	
25		60		95		130		165		200	
26		61		96		131		166		201	
27		62		97		132		167		202	
28		63		98		133		168		203	
29		64		99		134		169		204	
30		65		100		135		170		205	
31		66		101		136		171		206	
32		67		102		137		172		207	
33		68		103		138		173		208	
34		69		104		139		174		209	
35		70		105		140		175		210	
36		71		106		141		176		211	
37		72		107		142		177		212	
38		73		108		143		178		213	
39		74		109		144		179		214	
40		75		110		145		180		215	
41		76		111		146		181		216	
42		77		112		147		182		217	
43		78		113		148		183		218	
44		79		114		149		184		219	
45		80		115		150		185		220	
46		81		116		151		186		221	

m/e	Int.	m/e	Int.	m/e	Int.	m/e	Int.	m/e	Int.	m/e	Int.
222		262		302		342		382		422	
223		263		303		343		383		423	
224		264		304		344		384		424	
225		265		305		345		385		425	
226		266		306		346		386		426	
227		267		307		347		387		427	
228		268		308		348		388		428	
229		269		309		349		389		429	
230		270		310		350		390		430	
231		271		311		351		391		431	
232		272		312		352		392		432	
233		273		313		353		393		433	
234		274		314		354		394		434	
235		275		315		355		395		435	
236		276		316		356		396		436	
237		277		317		357		397		437	
238		278		318		358		398		438	
239		279		319		359		399		439	
240		280		320		360		400		440	
241		281		321		361		401		441	
242		282		322		362		402		442	
243		283		323		363		403		443	
244		284		324		364		404		444	
245		285		325		365		405		445	
246		286		326		366		406		446	
247		287		327		367		407		447	
248		288		328		368		408		448	
249		289		329		369		409		449	
250		290		330		370		410		450	
251		291		331		371		411		451	
252		292		332		372		412		452	
253		293		333		373		413		453	
254		294		334		374		414		454	
255		295		335		375		415		455	
256		296		336		376		416		456	
257		297		337		377		417		457	
258		298		338		378		418		458	
259		299		339		379		419		459	
260		300		340		380		420		460	
261		301		341		381		421		461	

m/e	Int.	m/e	Int.	m/e	Int.	m/e	Int.	m/e	Int.	m/e	Int.
462		502		542		582		622		683	
463		503		543		583		623		664	
464		504		544		584		624		665	
465		505		545		585		625		666	
466		506		546		586		626		667	
467		507		547		587		627		668	
468		508		548		588		628		669	
469		509		549		589		629		670	
470		510		550		590		630		671	
471		511		551		591		631		672	
472		512		552		592		632		673	
473		513		553		593		634		674	
474		514		554		594		635		675	
475		515		555		595		636		676	
476		516		556		596		637		677	
477		51/		557		597		638		678	
478		518		558		598		639		679	
479		519		559		599		640		680	
480		520		560		600		641		681	
481		521		561		601		642		682	
482		522		562		602		643		683	
483		523		563		603		644		684	
484		524		564		604		645		685	
485		525		565		605		646		686	
486		526		566		606		647		687	
487		527		567		607		648		688	
488		528		568		608		649		689	
489		529		569		609		650		690	
490		530		570		610		651		691	
491		531		571		611		652		692	
492		532		572		612		653		693	
493		533		573		613		654		694	
494		534		574		614		655		695	
495		535		575		615		656		696	
496		536		576		616		657		697	
497		537		577		617		658		698	
498		538		578		618		659		699	
499		539		579		619		660		700	
500		540		580		620		661		701	
501		541		581		621		662		702	

m/e	Int	m/e	Int.
703		743	
704		744	
705		745	
706		746	
707		747	
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710		750	
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